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Computer Sciences Corp., Research Triangle Park, NC

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DEVELOPMENT OF THE REGIONAL OXIDANT MODEL VERSION 2.1

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SECTION 1

INTRODUCTION

Although air quality levels in the United States for most criteria pollutants have improved over the past decade, harmful levels of photochemical smog still persist in many urban areas. Concentrations of ozone, a major component of photochemical smog, often exceed the air pollution standard established by the Clean Air Act. Implementing VOC and NO_x emission control programs can bring some areas closer to the primary ozone standard, but the effectiveness of control strategies must be evaluated before they are actually applied. Because mathematical modeling is a very powerful evaluation tool, the U.S. EPA has developed the Regional Oxidant Model (ROM) to predict the ozone concentration changes that would result from specified emissions changes for a given region.

Field studies have shown that ozone and its precursors can be transported more than 100 km from their point of origin. This indicates that the high ozone concentrations in many areas of the Northeast--particularly in areas of low emissions density--may be due in significant part to the influx of these species from outside sources. Thus, urban-scale models may be inadequate for evaluating ozone-reduction emissions scenarios because these models cannot accurately treat long-range transport of ozone and its precursors. The regional character of the ozone problem led the EPA to begin work on the first version of the ROM in the mid-1970s. The ROM is a sophisticated regional-scale model that predicts hourly ozone concentrations for episodes extending up to about a month in duration; each episode is modeled as a series of three-day executions. The model domain, composed of grid cells approximately 19 km by 19 km each, encompasses an area on the order of 1000 km by 1000 km. For much of eastern North America, the ROM can model the regional variability of the chemical and physical processes that affect photochemically-produced ozone concentrations on a regional scale:

- horizontal winds
- the photochemistry of airborne chemical species (including the nighttime chemistry of products and precursors of photochemical reactions)
- nocturnal jets and stable stratification
- cumulus cloud effects on vertical mass transport and photochemical reaction rates
- mesoscale vertical motion and eddy effects
- terrain effects on horizontal flows and on deposition and diffusion
- sub-grid-scale chemical processes (resulting from emissions from sources smaller than the model's grid can resolve)
- emissions of biogenic and anthropogenic ozone precursors
- dry removal processes (including the dry deposition of ozone)

The ROM system is composed of a core model, which solves the sets of equations that describe the above processes, and a series of over 30 processors that prepare the input data needed by the core model. ROM 1.0, the first version of the ROM, emerged in 1984 and was used for a limited set of applications for the Northeast Corridor Regional Modeling Project (Schere, 1986); refer to Lamb (1983), Lamb (1984), and Lamb and Laniak (1985) for more information on ROM 1.0. ROM 2.0 became operational in 1987. To create it from ROM 1.0, several features were changed or added: (1) The Demerjian chemical mechanism was replaced with version 4.0 of the Carbon Bond Mechanism (CBM 4.0) (Whitten and Gery, 1986), which simulates some 70 reactions among 28 chemical species. (2) Biogenic hydrocarbon emissions were added to the list of emission types modeled; ROM 1.0 modeled only anthropogenic emissions. (3) The code was modified to allow atmospheric layer thicknesses to vary over space and time; in ROM 1.0, these thicknesses remained constant. (4) The ability to simulate the effects of nocturnal jets and nighttime inversions was added.

Many different types of regulatory applications questions have been answered using ROM 2.0, as noted by Schere (1989). However, application requirements for EPA's Regional Ozone Modeling for Northeast Transport (ROMNET) project have prompted us to upgrade ROM 2.0 to produce ROM 2.1. For the ROMNET application, we have expanded the model's domain in the northeastern U.S. from 60 by 42 cells to 64 by 52 cells in order to include major urban emitters in Ohio and Virginia. As a result, the design of ROM 2.1 allows the user to increase or reduce the numbers of columns and rows in the grid more easily than before. ROM 2.1

also can be adapted more easily to other modeling domains in eastern North America. Some of the other modifications include an updated biogenic hydrocarbon processor; an improved wind fields processor; an upgraded Carbon Bond Mechanism (CBM 4.2) in the ROM's chemistry solver; expanded use of buoy data and the use of mobile-source emissions data; and changes that allow the ROM system to use computer resources more efficiently. We have also added features that should allow future outside users to apply the ROM more easily when it is released to them.

The changes and improvements made in creating ROM 2.1 are the subject of this report. In Section 2, we give a broad overview of the ROM, including a brief discussion of the ROM 2.1 processor network. Section 3 details some of the specific changes we made in upgrading the ROM 2.0 core model into the ROM 2.1 version; the core model currently resides on EPA-NCC's IBM® 3090. Changes to the input data processors, which reside on the EPA-NCC DEC VAX™ cluster, are discussed in Section 4. Finally, Section 5 summarizes the important differences between ROM 2.0 and ROM 2.1.

We hope that the reader will gain an appreciation for the complexity of the ROM system and will become familiar with some of the major technical and computer software improvements in this latest version of the ROM.

SECTION 2

OVERVIEW OF THE REGIONAL OXIDANT MODEL

The ROM is an Eulerian, episodic grid model that simulates the hourly concentrations of chemical species in a rectangular domain that is on the order of 1000 km on a side. The domain is represented by a grid of cells that are approximately 19 km on a side; the coordinate system that delineates the columns and rows of cells is based on the latitude-longitude system, so cell size varies somewhat over the domain. Columns are the north-south components of the grid (marked off in degrees longitude) and rows are the east-west components (marked off in degrees latitude). To date, the model has been adapted for three different regions (Figures 1a, 1b, and 1c): the Northeast Regional Oxidant Study (NEROS) region, consisting of 60 columns by 42 rows (2520 cells per atmospheric layer); the Southeast Regional Oxidant Study (SEROS) region (60 columns by 42 rows); and the Regional Ozone Modeling for Northeast Transport (ROMNET) region (64 columns by 52 rows, or 3328 cells per layer). ROM 2.0 has been applied in the NEROS and SEROS regions. ROM 2.1 has not yet been applied in any of these regions, but we have performed benchmark runs for the NEROS and ROMNET regions.

The ROM has three and one-half vertical layers--termed layers 0, 1, 2, and 3--whose thicknesses vary dynamically in space and time in response to meteorological phenomena (Figure 2). Layers 1 and 2 encompass most of the planetary boundary layer, layer 3 is the cloud or capping inversion layer extending from cloud base to near the tops of any cumulus-type clouds, and layer 0 is a shallow surface layer designed to parameterize surface deposition and sub-grid-scale effects on chemical reaction rates due to spatially-heterogenous emissions distributions. The height of the domain (the height of layer 3's top) varies between about 600 m above mean sea level (MSL) and about 4500 m above MSL. We say there are three and one-half layers rather than four because in layers 1, 2, and 3 the concentrations of chemical species are treated prognostically, while in layer 0 they are treated diagnostically.

For each model layer, the ROM system combines observational data and theoretical formulations of the governing chemical and physical processes to produce predicted species concentrations. The main component of the system, the core model, is a set of algorithms that calculate the solutions to computer-solvable analogues of the differential equations that describe the governing processes. The core model outputs concentrations for all species for every cell in every layer, for each model time step. The basic model time step, called the advection time step, is one-half hour. Within each advection time step, the vertical fluxes and chemical kinetics are modeled using smaller time steps. A single core model run can simulate episodes up to 72 hours (144 advection time steps) in length; this limit is imposed because of file-size restrictions. Episodes of longer than three days are run as a series of 72-hour executions; simulations usually are limited to the length of an ozone episode (approximately two weeks).

The core model requires five types of input data: air quality, meteorology, emissions, land use, and topography. We acquire these raw data from various sources and process them through data extraction and quality assurance routines. This process produces data that are then prepared for the core model by a network of over 30 processors, which range in function from simple data reformatting routines to programs that generate the complex wind fields that drive the atmospheric transport. The processors are organized into nine distinct stages that reflect the sequence of program execution. Processors at the same stage may execute simultaneously, but each processor must wait to execute until all the lower-stage processors in its data path have finished running.

Most of the processors in the network produce either processor files (PFs) or model files (MFs). PFs, generally output by lower-stage processors, contain data used by higher-stage processors. MFs also provide input to some higher-stage processors, but they primarily contain the parameter fields that are transformed into the data elements required by the core model governing equations. The processor network ultimately produces several large data files for the core model, which contain initial-condition and boundary-condition concentrations as well as the data used to model all physical and chemical processes affecting species concentrations in a given episode. These files combined contain tens of millions of core model input values; simulating one day, for example, requires nearly 100 billion computations with these millions of values.

Figure 3 is a schematic of the ROM system. By structuring the ROM in this modular fashion, we can change the method used to generate values of a particular independent variable without having to overhaul the entire ROM system. Thus, to create ROM 2.1 from ROM 2.0, we have been able to modify and improve some

components without having to rewrite the code for all the others. Figure 4 shows the resulting ROM 2.1 processor network. It consists of three interrelated parts: the initial-condition and boundary-condition (IC/BC) processors; the meteorology processors, which process topography and land use data in addition to meteorology data; and the emissions processors. The network transforms the raw data input files into the four core model input files shown on the far right: ICON (initial-condition concentration data), BCON (boundary-condition concentration data), BTRK [diffusivity and backtrack (advection transport) information], and BMAT (parameterization for vertical fluxes, meteorological parameters necessary for chemistry rate constant adjustments, and parameterized emissions source strengths). Table 1 summarizes the functions of all the processors in the ROM 2.1 network.

The modular structure is also advantageous because it facilitates implementing quality assurance (QA) procedures. All programs in the system are operated and maintained in strict conformance with a set of QA procedures that involve both machine and human checks of the computer code, the input and output data streams of each submodule, and the overall behavior of the model.

The ROM system has been programmed using the American National Standards Institute (ANSI) FORTRAN-77 full language specification, except for the Biogenic Emissions Inventory System (BEIS), an emissions processing system written in SAS®. Development of the system began on the EPA's Sperry UNIVAC® 1100 mainframe computer. It was then shifted to a VAX 11/780 minicomputer in May 1983. Currently, we are running the core model on the EPA-NCC's IBM 3090 and the processor network on the EPA-NCC VAX cluster, consisting of two VAX 8650s and one VAX 11/785. Running the model system requires a significant amount of CPU time; for example, for one three-day execution, the ROM 2.0 core model required about 6 h of IBM 3090 CPU time and the ROM 2.0 processor network used about 12 h of VAX 8600 CPU time.

Throughout the implementation and enhancement of the ROM, emphasis has been placed on using the Jackson Structure Programming method (Jackson, 1975) and the Jackson System Development method (Jackson, 1983). These methods provide a clear description of the overall organization, understandable dynamic documentation, maintainable programs, and standardization of software design.

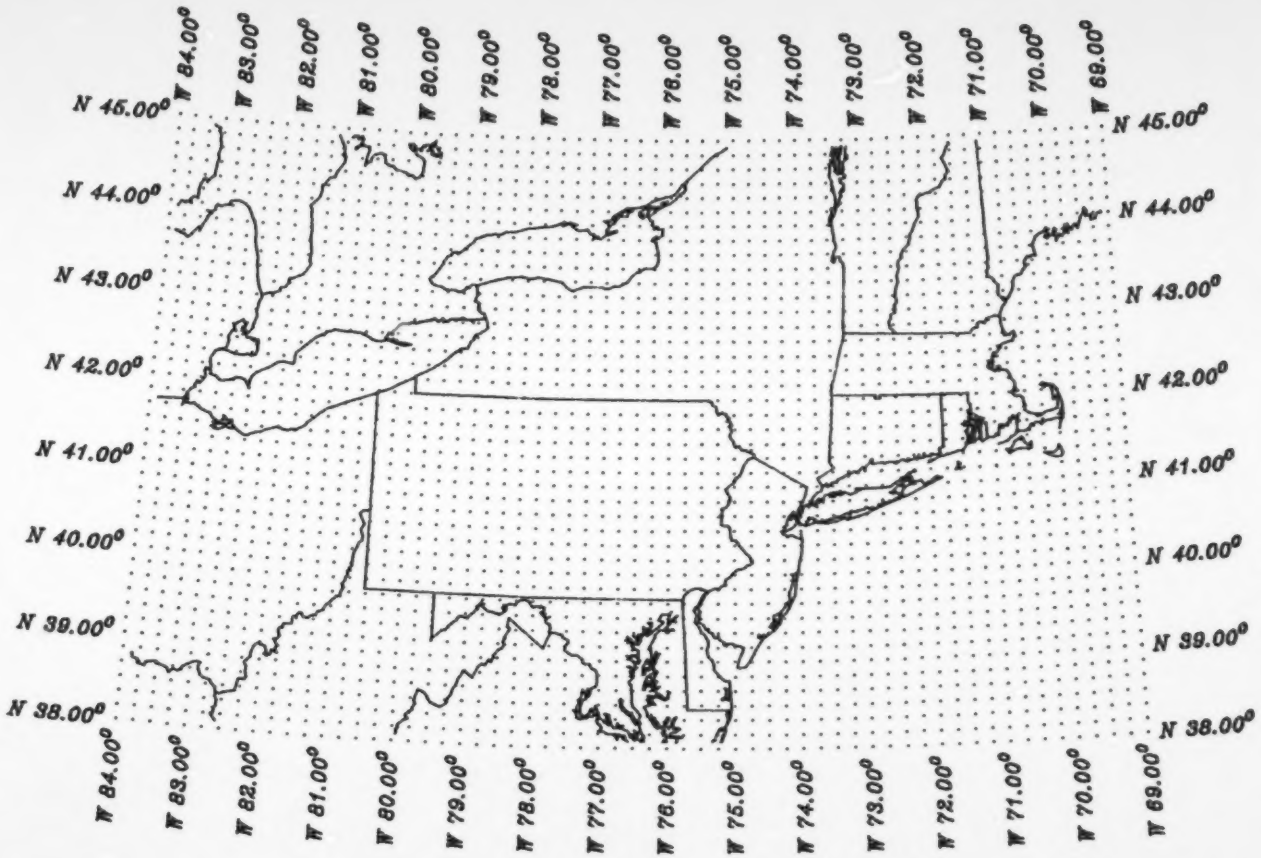

Figure 1a. The gridded NEROS region (60 columns by 42 rows); dots represent grid cell corners.

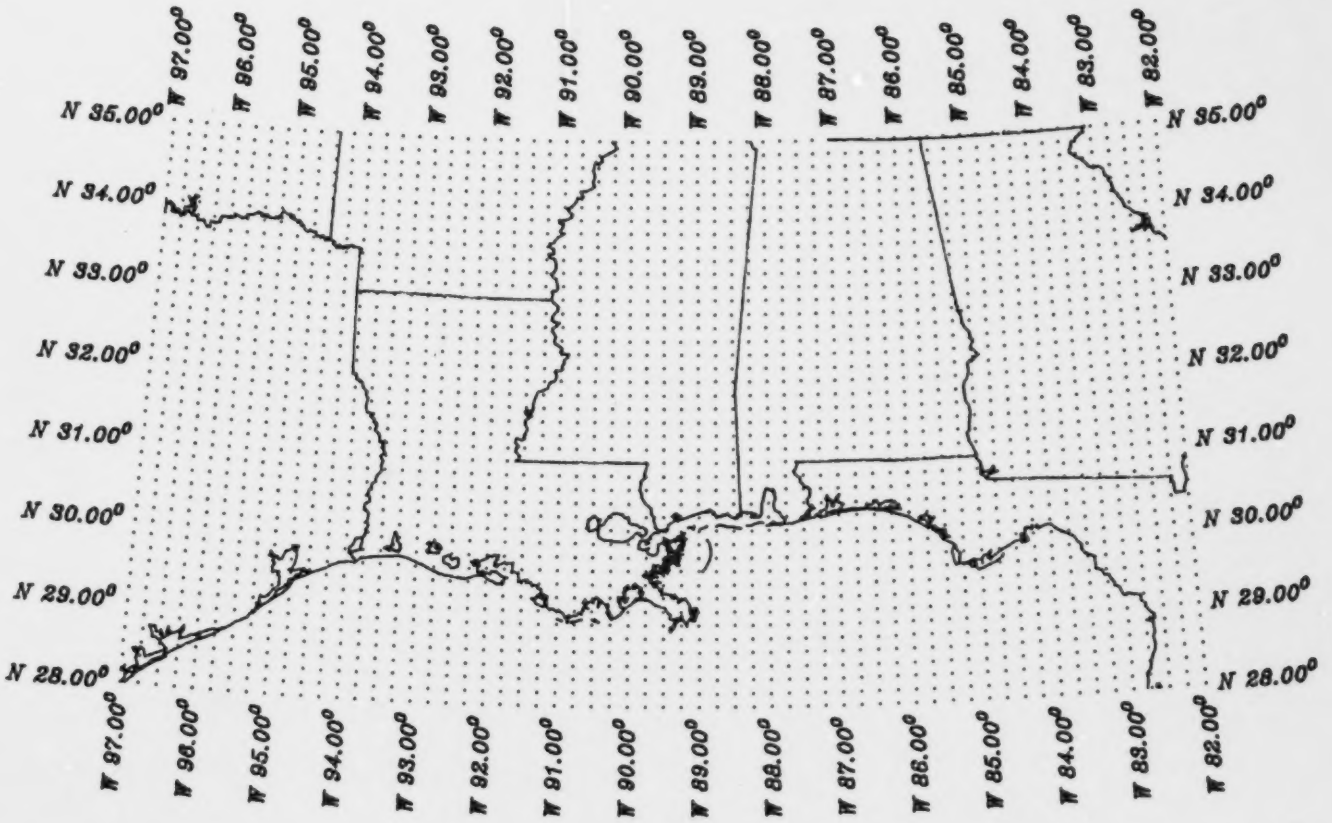

Figure 1b. The gridded SEROS region (60 columns by 42 rows); dots represent grid cell corners.

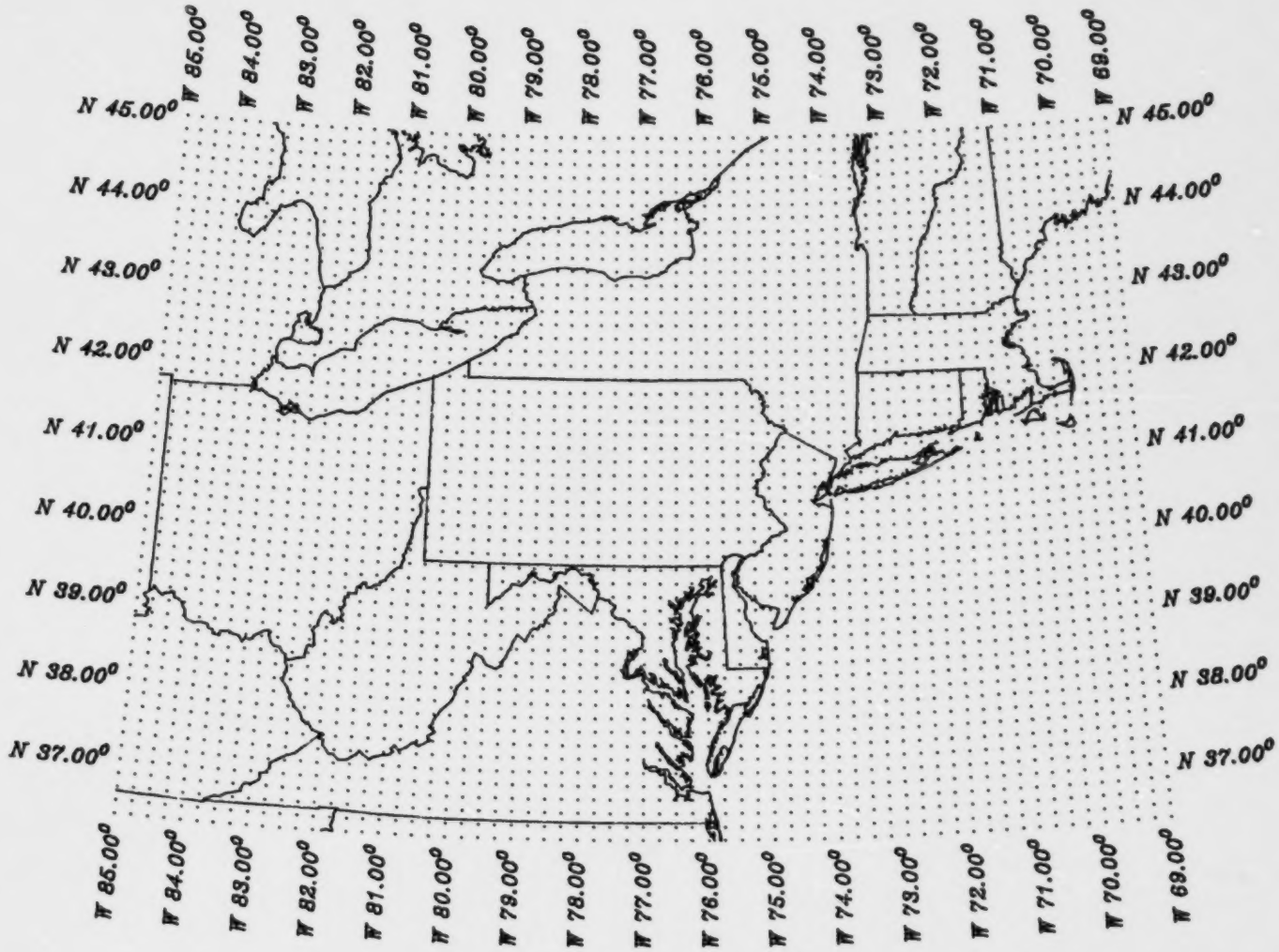

Figure 1c. The gridded ROMNET region (64 columns by 52 rows); dots represent grid cell corners.

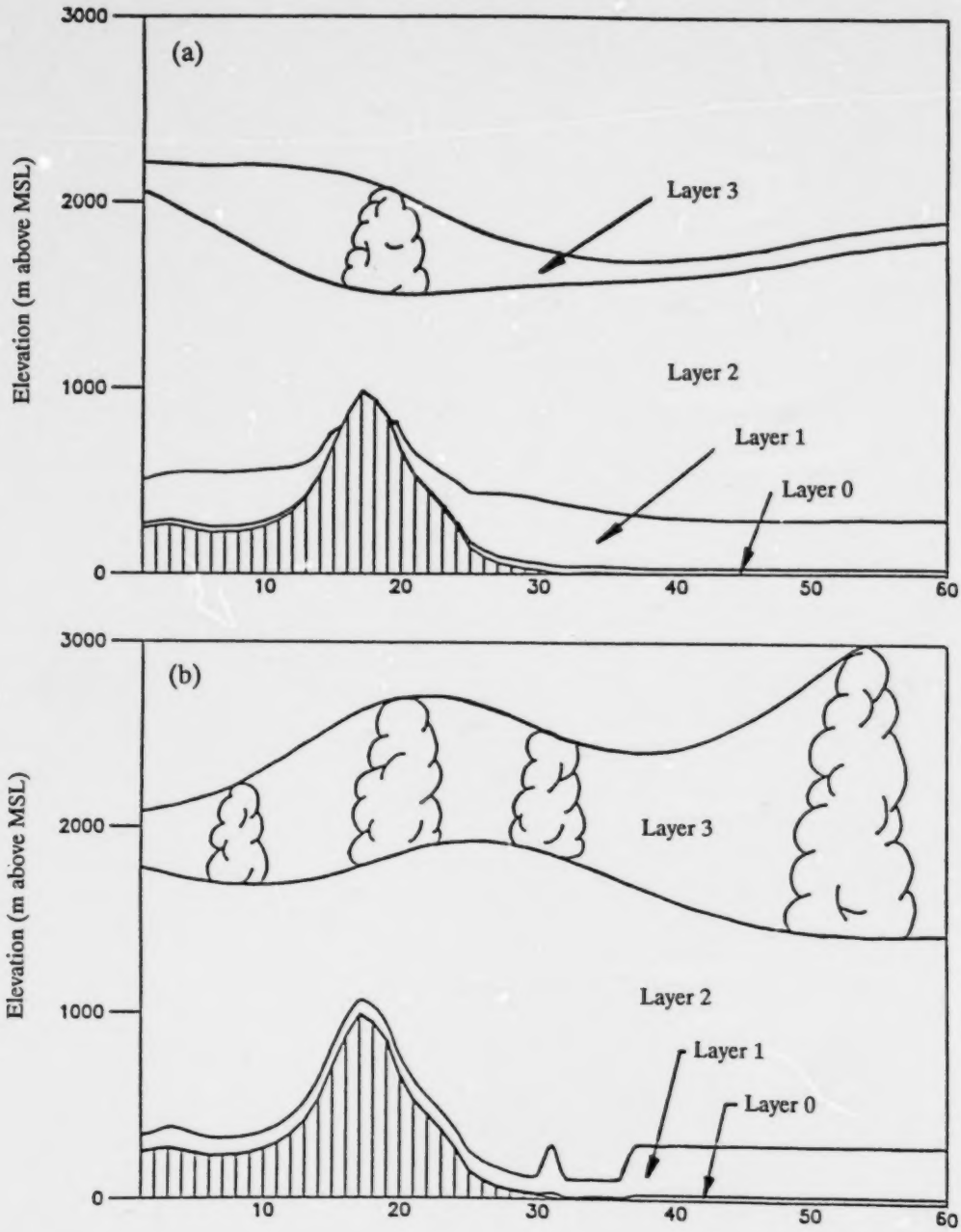

Figure 2. Cross-section through ROM model layers along latitude 38° 40′ at (a) hour 0700 EST and (b) hour 1000 EST, on July 18, 1980. Numbers along abscissa denote grid column.

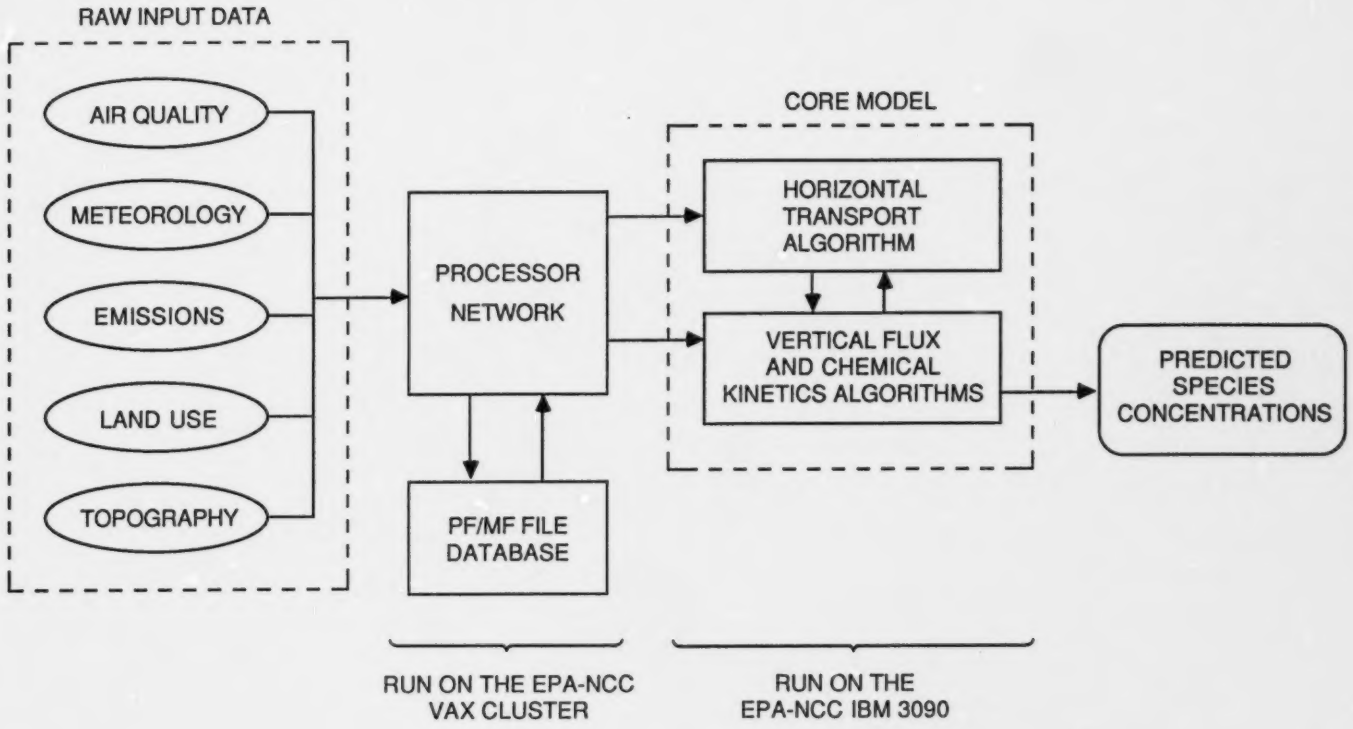

Figure 3. General structure of the ROM system, from input data through final output concentrations

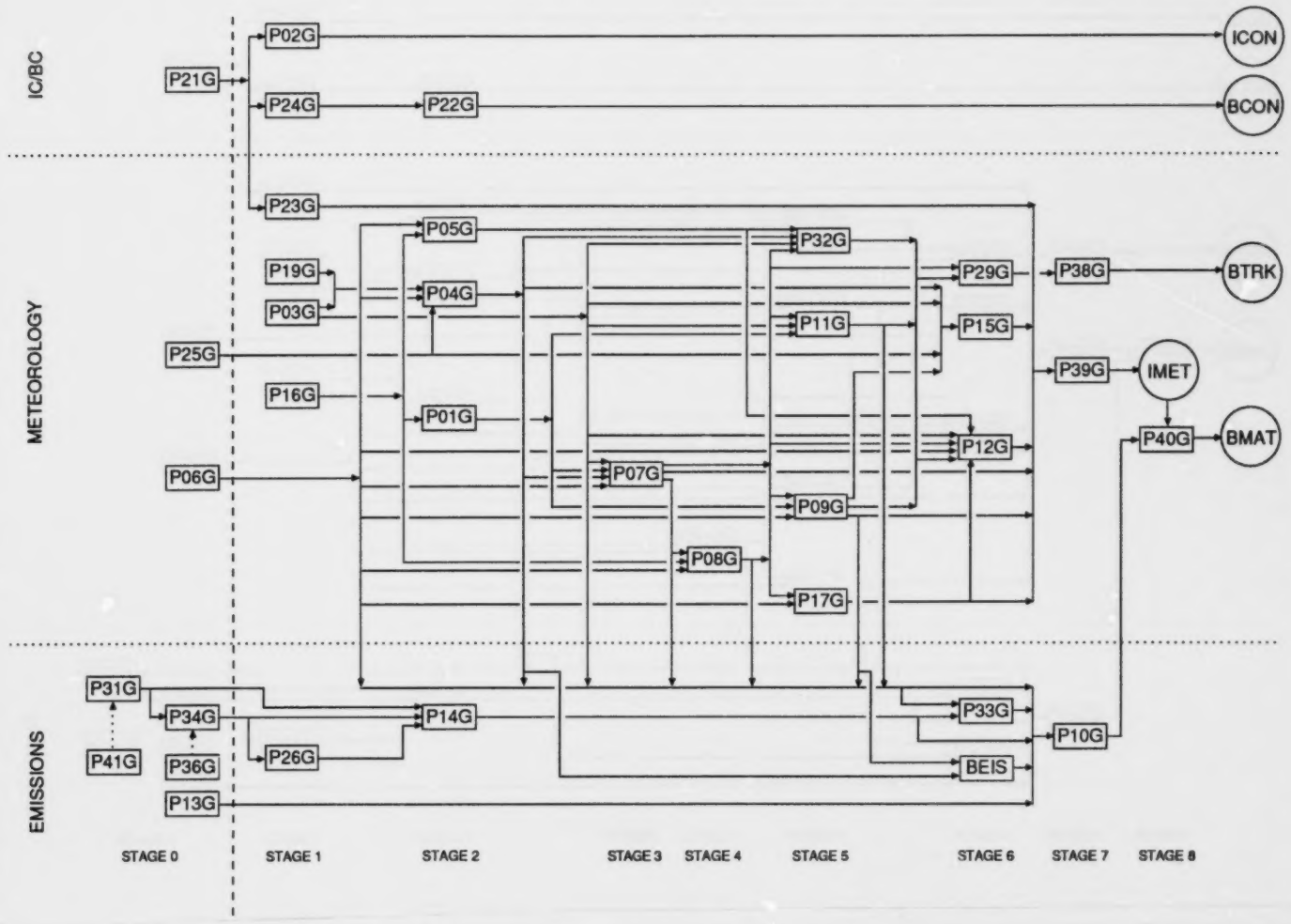

Figure 4. Structure and output files of the ROM 2.1 input processor network.

TABLE 1. FUNCTIONAL DESCRIPTIONS OF THE ROM 2.1 INPUT PROCESSORS

Processor	Stage	Function in ROM 2.1
P01G	2	Interpolates profiles of upper-air meteorological parameters at intervals of 50 m from hourly rawinsonde vertical profiles
P02G	1	Writes to the file ICON the gridded initial-condition concentrations for each layer and species simulated by the core model, using P21G's clean-air concentrations as initial-condition concentrations
P03G	1	Prepares surface meteorology data (e.g., mixing ratio, virtual temperature, and wind speed) for use in higher-stage processors
P04G	2	Computes gridded surface roughness, and hourly gridded Monin-Obukhov length, surface heat flux, friction velocity, surface temperature, surface relative humidity, and surface wind speed
P05G	2	Uses surface observations to compute hourly gridded values for the fraction of sky covered by cumulus clouds, and also calculates cumulus cloud-top heights
P06G	0	Computes the smoothed terrain elevation for each 10′ lat. by 15′ long. ROM domain grid cell, and also for a larger domain that extends three grid cells beyond the ROM domain. In addition, it computes average terrain elevations in a finer-resolution domain (cells 5′ lat. by 5′ long.) for the terrain penetration calculation. Finally, it computes the north-south and east-west components of the terrain elevation gradient (slope)
P07G	3	Computes hourly gridded wind fields in the cold layer, hourly gridded terrain penetration fractions, hourly gridded cold layer growth rates, and hourly gridded thicknesses for layers 0 and 1
P08G	4	Computes hourly gridded cell thicknesses for layers 2 and 3, and various parameters used to specify volume fluxes between these two layers
P09G	5	Computes hourly gridded atmospheric density, temperature, cloud cover, solar zenith angle, and water vapor concentration
P10G	7	Computes hourly gridded emissions source functions in layers 0, 1, and 2 for combined anthropogenic and biogenic sources, and also computes the plume volume fraction in layer 0
P11G	5	Computes hourly gridded horizontal winds for each layer, using rawinsonde vertical profiles and surface-station wind observations

(continued)

TABLE 1. (CONTINUED)

Processor	Stage	Function in ROM 2.1
P12G	6	Computes hourly gridded volume fluxes through all model layer boundaries, and cumulus cloud vertical flux parameters
P13G	0	Computes the total length of all line emissions sources (highways and railroads) within each grid cell
P14G	2	Prepares files containing hourly emissions values and stack descriptions for all major point sources, and combined hourly gridded emissions values for minor point sources, area sources, and mobile sources
P15G	6	Computes hourly gridded effective deposition velocities for a set of representative species
P16G	1	Interpolates between rawinsonde observations to produce hourly upper-air profiles at 25-mb resolution
P17G	5	Computes hourly gridded elevations (above MSL) for the tops of layers 0, 1, 2, and 3, and local time derivatives of these elevations
P19G	1	Computes hourly gridded values of fractional sky coverage at the terrain surface for all cloud types combined
P21G	0	Computes daytime and nighttime tropospheric background (clean-air) concentrations in each layer for each chemical species
P22G	2	Computes and writes to the file BCON the gridded boundary-condition concentrations for each species, layer, and advection time step simulated by the core model, for the north, south, east, and west boundaries
P23G	1	Computes hourly gridded upper-boundary-condition concentrations (C-infinity) for a set of representative species
P24G	1	Equilibrates background concentrations of all modeled chemical species with averaged observed ozone concentrations on the north, south, east, and west boundaries, for both daytime and nighttime conditions in each layer
P25G	0	Computes the fraction of each grid cell in each land use category recognized by the model

(continued)

TABLE 1. (CONCLUDED)

Processor	Stage	Function in ROM 2.1
P26G	1	Computes hourly gridded mobile-source VOC, NO_x, and CO emissions parameters, adjusted for daily average temperature
P29G	6	Computes hourly gridded 30-min backtrack (advection) cell locations and horizontal diffusivities for each layer simulated by the core model
P31G	0	Allocates annual point-source emissions data between a weekday-emissions file, a Saturday-emissions file, and a Sunday-emissions file
P32G	5	Calculates hourly gridded horizontal eddy diffusivities for layers 1, 2, and 3, and also produces parameter fields needed to compute interfacial volume fluxes across layer boundaries
P33G	6	Generates hourly gridded locations and strengths of constant-source emitters for a tracer emissions species
P34G	0	Converts all point-, area-, and mobile-source data files from GMT to LST
P36G	0	Applies NO_x and VOC emission controls at the county level for area- and mobile-source emissions data
P38G	7	Reads the backtrack and diffusivity hourly gridded MF files and computes the BTRK file parameters for each advection time step simulated by the core model
P39G	7	Reads all meteorology hourly gridded MF files *except* the backtrack and diffusivity files read by P38G and computes the intermediate meteorology (IMET) file parameters for each advection time step simulated by the core model
P40G	8	Reads the intermediate meteorology (IMET) file and the emissions sources hourly gridded MF files and computes the BMAT parameters for each advection time step simulated by the core model
P41G	0	Applies NO_x and VOC emission controls to point-source emissions data, at a state, county, point, or individual-boiler level
BEIS*	6	Prepares hourly gridded biogenic emission rates for isoprene, paraffin, olefin, high molecular weight aldehydes (RCHO, R > H), nonreactive hydrocarbons, NO, and NO_2, based on a canopy model

*All processors (PnnG) are written in FORTRAN, but the Biogenic Emissions Inventory System (BEIS) is written in SAS. Because of this difference, the BEIS is not given a PnnG name.

SECTION 3

CHANGES TO THE CORE MODEL AND ITS INPUT FILES, INCLUDING CHANGES THAT SHOULD ALLOW FUTURE OUTSIDE USERS TO APPLY THE CORE MODEL

As explained in Section 2, the core model is the ROM component that predicts final concentrations for all species modeled, based on data in several large input files produced by the processor network. The core model calculates the solution to computer-solvable analogues of the differential equations that describe the governing chemical and physical processes in each model layer. In simplest terms, for each Carbon Bond Mechanism species in each layer, the core model solves the basic diffusion equation for c, the species concentration in volumetric units (ppm). The implementation decomposes c as

$$c = \Gamma \cdot \gamma$$

in order to form differential equations to compute Γ and γ, where Γ represents the component of the concentration due to horizontal transport and diffusion and γ represents the component due to chemical kinetics and vertical fluxes across layer boundaries. Following the form of the differential equations, the core model is logically composed of two major modules, BIGGAM and LILGAM [referring to Γ and γ, respectively; for further details on the core model's theoretical formulation, please refer to Lamb (1983)]. BIGGAM consists of the horizontal transport algorithm and LILGAM consists of the vertical flux and chemical kinetics algorithms. These modules are shown (although not by name) in Figure 3. There are also a number of smaller modules that process data needed by BIGGAM and LILGAM.

This section discusses the changes we made to the ROM 2.0 core model in order to create the ROM 2.1 version. Section 3.1 details the changes made to the core model itself, including changes to the ROM chemistry solver, core model I/O changes to improve efficiency, and miscellaneous minor modifications. Section 3.2 covers changes made to the ROM 2.1 core model that should help future out-of-house users apply it.

3.1 CHANGES TO THE CORE MODEL AND ITS INPUT FILES

3.1.1 ROM Chemistry Solver Changes

The LILGAM module in the core model includes the ROM chemistry solver, a set of algorithms that model oxidant chemical kinetics. For ROM 2.1, we made three major changes to this solver: the version of the Carbon Bond Mechanism was changed, the FRAX control mechanism was altered, and methanol was added to the species list. The first two changes caused a sizable increase in computation time, relative to ROM 2.0. For the NEROS domain, the ROM 2.1 core model consumes approximately 9.25 h of IBM 3090 CPU time for a three-day execution, or about 54% more time than ROM 2.0's core model.

3.1.1.1 Changing the Version of the Carbon Bond Mechanism--

The ROM solver in ROM 2.0 was based on Carbon Bond Mechanism 4.0 (CBM 4.0) (Whitten and Gery, 1986). In ROM 2.1, the solver is based on CBM 4.2 (Gery et al., 1988), an upgraded version of CBM 4.0. We have modified the solver to reflect the differences between these two versions, which fall into three major categories:

(1) The CBM 4.2 species list differs from CBM 4.0's list. In creating the ROM 2.1 version of CBM 4.2 from the ROM 2.0 version of CBM 4.0, nine species were added to the list and four dropped from it; overall, the total number of species increased from 30 to 35. Table 2 lists all the chemical species for both CBM 4.2 and CBM 4.0.

(2) The list of chemical reactions describing the rates of production and destruction of individual chemical species has also changed, primarily because of the altered species list. In ROM 2.0, there were 72 reactions; in ROM 2.1, there are 83. The changes in the reaction list also required us to modify the list of reaction rate constants.

TABLE 2. CHEMICAL SPECIES LISTS FOR CBM 4.2 AND CBM 4.0

Species common to both CBM 4.2 and CBM 4.0	Species in CBM 4.2 only	Species in CBM 4.0 only
High molecular weight aldehydes (RCHO, R > H)	Cresol and higher molecular weight phenols	Phenol (cresol) surrogate (aromatic-OH)
Peroxyacyl radical [$CH_3C(O)O_2$]	High molecular weight aromatic oxidation ring fragment	Phenoxy radical surrogate (aromatic-O)
Carbon monoxide (CO)	O^1D atom (singlet)	Methane (CH_4)
Ethene ($CH_2=H_2C$)	Methylphenoxy radical	Tolualdehyde ($CH_3C_6H_4CHO$)
Formaldehyde (CH_2O)	Peroxynitric acid (HO_2NO_2)	
Hydrogen peroxide (H_2O_2)	Secondary organic oxy radical	
Nitrous acid (HNO_2)	Toluene-hydroxyl radical adduct	
Nitric acid (HNO_3)	Methanol (CH_3OH)	
Hydroperoxy radical (HO_2)	Tracer species	
Isoprene [$CH_2=C(CH_3)CH=CH_2$]		
Methylglyoxal [$CH_3C(O)C(O)H$]		
Dinitrogen pentoxide (N_2O_5)		
Nitric oxide (NO)		
Nitrogen dioxide (NO_2)		
Nitrogen trioxide (NO_3)		
O^3P atom (triplet)		
Ozone (O_3)		
Hydroxyl radical (OH)		
Olefinic carbon bond (C=C)		
Peroxyacyl nitrate [$CH_3C(O)O_2NO_2$]		
Paraffinic carbon bond (C-C)		
Toluene ($C_6H_5CH_3$)		
NO-to-NO_2 operation		
NO-to-nitrate operation		
Xylene ($C_6H_4(CH_3)_2$)		
Nonreactive hydrocarbons		

(3) We changed the way the reaction rate constants are adjusted. In ROM 2.0, reaction rate constants were adjusted using just temperatures and air densities representative of each layer (for both daytime and nighttime conditions). ROM 2.1 uses a third variable, water vapor concentration, to adjust some of the rate constants.

3.1.1.2 New FRAX Control--

The ROM solver arrives at solutions by iterating through a series of variable-length time steps called chemistry time steps (CTSs). The length of any CTS must lie between fixed upper and lower limits, called BLIM and ULIM in the code; in ROM 2.0, BLIM was equal to 10 s and ULIM was equal to 60 s. Within these limits, the length of a CTS is inversely proportional to the degree of "stiffness" of the ROM solver chemistry system. A relatively stiff system is one in which the chemical species are not in equilibrium at the beginning of each advection (half-hour) time step. The stiffer--or farther out of equilibrium--the system is, the shorter the CTS must to be in order to achieve the same degree of accuracy. However, each CTS also must be as long as possible so that computation time is not excessive. To reconcile these two competing needs, the ROM solver determines CTS length using an adjustable control parameter called FRAX.

FRAX is assigned one of two values, based on the value of a solver tolerance parameter called FRACNO. The model determines the value of FRACNO by comparing the newly-computed nitric oxide (NO) concentrations for the current CTS with the NO concentration values already calculated for the previous CTS; the larger the fractional difference (i.e., the stiffer the system), the larger the FRACNO value. The model then compares FRACNO with a constant-value parameter called FNOLIM. If FRACNO is greater than FNOLIM, the lower FRAX value is chosen. Thus, in regions where the ROM solver equation system is stiffer, or farther out of equilibrium (for example, in cells containing higher emissions), the value of FRACNO is more likely to exceed the value of FNOLIM, so the lower FRAX value is used and the CTS is shorter. The value of FRACNO is based on NO because this species provides the best index of the chemical reaction system's overall activity.

In ROM 2.1, we have decreased the value of FNOLIM by a factor of 60, in part because the CBM 4.2 system is stiffer than the CBM 4.0 system. Thus, FRACNO is larger than FNOLIM much more often, so shorter CTSs are more frequent. However, this significantly increases model

computation time. To help lessen this time penalty, we increased the value of BLIM, the minimum allowable CTS length. Box model tests we conducted indicated that BLIM could be relaxed from 10 s to 20 s without incurring a significant loss in solution accuracy, so in ROM 2.1 BLIM is equal to 20 s.

3.1.1.3 Inclusion of Methanol--

ROM 2.1 can include methanol in its ROM solver reactions, if desired; ROM 2.0 did not model this species. Methanol can be included in the modeling process in order to evaluate ozone-reduction strategies involving choices between automotive fuels.

3.1.2 Core Model I/O Modifications to Improve Efficiency

3.1.2.1 Redesign of the B-Matrix File--

In ROM 2.0, the core model required three large input files, produced by the processor network: IC, which contained initial-condition species concentration data for the entire grid; BC, which contained boundary-condition species concentration data for all the grid boundaries; and BMAT, or the B-matrix file, which contained (1) parameterization for vertical fluxes, (2) horizontal transport parameters, (3) meteorological parameters necessary for chemistry rate constant adjustment, and (4) parameterized emissions source strengths. These data are needed by the BIGGAM and LILGAM modules in the core model, and are in a form related specifically to the form of the core model's generalized finite difference algorithms.

For ROM 2.1, the forms of the initial-condition file (now called the ICON file) and the boundary-condition file (now called the BCON file) are the same as for ROM 2.0. However, we decided to split the 2.0 B-matrix file into two files for ROM 2.1: the BTRK file and the new BMAT file. Because the combined file is extremely large and because BIGGAM's and LILGAM's data requirements do not overlap, it is more efficient from an I/O standpoint to contain each module's input data in a separate file. The BTRK file contains the diffusivity and backtrack (advection transport) data required by BIGGAM. The new BMAT file contains the data needed by LILGAM and its subroutines for interlayer mass flux adjustments and for adjustments to the chemical reaction rate constants.

After we split the old BMAT file, we also redesigned the new BMAT file to be what is called a multiple BMAT file--a sequence of files that can be distributed over many disks. With the increase to 35 chemical species and the move to larger grid domains, a ROM 2.1 BMAT file for a full three-day execution might not fit on the major VAX mass storage devices currently used on the EPA-NCC cluster. The multiple BMAT design not only alleviates that problem but also allows more efficient use of disk space, because a multiple BMAT file can be distributed over many disks that are already partially filled.

3.1.2.2 Redesign of the Intermodule Communication System--

As we redesigned ROM 2.0 to create ROM 2.1, two changes we made allowed us to increase the efficiency of the intermodule communication (I/O) system within the core model. First, we divided the ROM 2.0 B-matrix file into two ROM 2.1 files (BTRK and the new BMAT), as discussed above. Second, we eliminated the row-windowing feature in ROM 2.0's BIGGAM module. Implemented previously because of memory limits on older computers, this feature allowed the model to split up its computational grid and move only a limited portion into core memory at any one time. Because current CPUs have much higher memory limits, we have removed this row-windowing feature to improve efficiency. This feature also hampered the development of a ROM multiprocessor prototype being built through a cooperative agreement between the EPA and Research Triangle Institute.

These two changes led us to implement BIGGAM as the "main" program; as such, it took over the functions of ROM 2.0's SUPERV main routine, which supervised communications between modules. Also, we simplified and renamed (from RUNSCHDL to RUNMGR) the core model driver used to facilitate execution restarts after partial simulation completions.

3.1.3 Miscellaneous Core Model Modifications

We made several other changes to the ROM 2.0 core model in creating the ROM 2.1 version:

- In ROM 2.0, BIGGAM computed grid values in vertical-layer-then-column order; in other words, it computed values for all columns in a layer before moving on to the next layer. For ROM 2.1, we reversed this order to facilitate developing Research Triangle Institute's ROM multiprocessor prototype.
- We improved reporting to the run-time log file.

- We standardized the code so that it is easier to read and to maintain.
- We simplified and standardized the structure of the file headers that give information on the contents of each file.

3.2 CHANGES THAT SHOULD ALLOW FUTURE OUTSIDE USERS TO APPLY THE CORE MODEL[1]

As the ROM system evolves into a practical applications tool, we anticipate that other organizations will want to use it. Therefore, we have designed the ROM 2.1 core model and parts of the processor network to be more accessible to outside users.

To run the core model, four input files are needed: the initial-condition (ICON) file (from processor P02G); the boundary-condition (BCON) file (from processor P22G); the backtrack (BTRK) file (from processor P38G); and the B-matrix (BMAT) file (from processor P40G), which includes both meteorology and emissions data. We envision that future users will be able to process their own emissions data by running stages 0 through 5 of the emissions processors for each emissions scenario they choose to model. We plan eventually to release all emissions processors to the outside user community with appropriate documentation.

With later releases of the ROM, we anticipate that after processing their own emissions data as described above, users will then run stages 0 through 7 of the meteorology processors and also complete stages 6 and 7 of the emissions processors (using as input the few required meteorology processor output files). Finally, the users will run processor P40G in stage 8 to combine emissions and meteorology data and create a BMAT file. Currently, however, having outside users run the meteorology portion of the network would impose too large an ADP burden on them. Furthermore, processing correctly all the raw meteorology data needed by P40G requires a massive amount of specialized work by trained personnel.

As a result, we have designed stages 0 through 7 of the ROM 2.1 meteorology processors to produce for each three-day ROM execution an intermediate meteorology (IMET) file (see Figure 4), which we can create in-house and provide to outside users. We will also provide the few meteorology processor output files they need to run the emissions processors P33G and P10G. With our IMET file and their emissions output files, the users will then be able to run processor P40G and produce their own BMAT file.

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[1] You will find this section much easier to follow if you have Figure 4 (from Section 2) in front of you as you read.

For each episode the users request, we will also create and provide the other three core model input files: BTRK, ICON, and BCON. By combining these with the BMAT file they have created, outside users will be able to run the core model with whatever emission control strategies they choose.

SECTION 4

CHANGES TO THE INPUT PROCESSOR NETWORK

As discussed in Section 2, the core model requires five types of input data--air quality, meteorology, emissions, land use, and topography--that are prepared for the core model by a network of over 30 processors (see Figure 4 and Table 1 in Section 2). These processors are organized in nine distinct stages that reflect the sequence of program execution; processors at the same stage may execute simultaneously, but each processor must wait to execute until all the lower-stage processors in its data path have finished running.

Most of the processors in the network produce either processor files (PFs) or model files (MFs). PFs, generally output by lower-stage processors, contain data used by higher-stage processors. MFs also provide input to some of the higher-stage processors, but they primarily contain the parameter fields that are transformed into the input variable values required by the core model algorithms. The processors use specially-designed software to access the PFs and MFs; information contained in a file called the PF/MF database directory file controls the processors' access. The directory file contains a main header that briefly defines the application parameters, and a record entry for each PF or MF used. The database header and records describe files whose content is specific to a particular region (e.g., grid dimensions, PF/MF numbering scheme), so there must be a unique database for every region and/or application.

The processor network ultimately produces the large data files used as input by the core model. In ROM 2.1, these files are the ICON file, the BCON file, the BTRK file, and the BMAT file, all discussed in Section 3.

This section discusses the changes made to the processor network in converting ROM 2.0 to ROM 2.1. It is divided into three major subsections: generic changes made to many or all of the processors (Section 4.1),

specific changes made to individual processors (Section 4.2), and changes made to the PF/MF database (Section 4.3). In addition to the changes listed in the next sections, the code for all processors and the PF/MF database was standardized for ROM 2.1 so that it is easier to read and to maintain. Also, refer back to Section 3.2 for information on how the ROM 2.1 processor network has been designed to produce an intermediate meteorology (IMET) file to facilitate releasing the core model to outside users.

4.1 GENERIC CHANGES THAT AFFECTED MANY PROCESSORS

4.1.1 Changes in Domain Size and Location

As discussed in Section 2, the ROM domain is a rectangular area that is on the order of 1000 km on a side, marked off into columns and rows of grid cells based on the latitude-longitude system; individual grid cells are approximately 19 km by 19 km. In ROM 2.0, the only grids we used were 60 columns by 42 rows. When we created ROM 2.1, we completed enhancements that allow us to apply the model to domains with other dimensions. This development was prompted by the ROMNET project, for which we expanded the grid to 64 columns by 52 rows. Because of VAX/VMS™ FORTRAN limitations and the PF/MF database structure, however, the number of columns times the number of rows times the number of parameters per I/O file must not exceed 65,535. Thus, for the ROMNET grid, we are limited to nineteen parameters per I/O file. If we add more parameters, we will have to make major changes to the PF/MF database and the I/O utilities.

In addition, we have modified the entire processor network and the core model so that we can apply the ROM more easily to different geographic regions, although assumptions made as we developed the theoretical basis for the ROM limit the regions of applicability to domains mainly within the U.S., excluding the Rocky Mountain region and large data-sparse regions (e.g., domains containing mostly ocean).

4.1.2 Changes in the Chemical Kinetics Implementation

Two of the three ROM chemistry changes explained in Section 3 also affected some of the existing processors for ROM 2.1. These changes are discussed here in general terms because they affect a number of processors; we will explain the modifications more thoroughly in Section 4.2.

4.1.2.1 Changing the Version of the Carbon Bond Mechanism--

As noted in Section 3.1.1.1, the implementation of ROM 2.1's CBM 4.2 differs from ROM 2.0's CBM 4.0 in three areas: the list of chemical species, the list of chemical reactions, and the way in which chemical reaction rate constants are adjusted. Changing the species list (see Table 2 in Section 3) meant that we had to modify all existing ROM 2.0 IC/BC processors (P02G, P22G, P23G, and P24G) to create the ROM 2.1 versions. The updated species list was also included in the new processor P21G.

Changes in the list of reactions, caused mainly by changing the species list, affected two ROM 2.0 IC/BC processors: P23G and P24G. These processors (as well as ROM 2.1's P21G) include a set of algorithms called GPRIME that is based on the same ROM chemistry solver mechanism used in the core model's LILGAM module; as a result, we had to change these processors in the same ways we altered the core model to include the new reaction list (see Section 3).

In addition, we modified processor P09G to reflect the addition of water vapor concentration to the list of variables used in adjusting the CBM 4.2 reaction rate constants.

4.1.2.2 Adding Methanol to the Species List--

As discussed in Section 3.1.1.3, ROM 2.1 can process the emission species methanol. Adding methanol to the species list required modifying the code of five of the existing ROM 2.0 emissions processors to accept an additional species: P10G, P14G, P31G, P33G, and P34G.

4.2 SPECIFIC CHANGES TO INDIVIDUAL PROCESSORS

The information in this section is divided into three main subsections, based on the processor network groupings shown in Figure 4 (Section 2): IC/BC processors (Section 4.2.1), meteorology processors (Section 4.2.2), and emissions processors (Section 4.2.3). Within each subsection, processors are presented in stage order (lowest stage to highest), and within stage groups in ascending numeric order.

4.2.1 IC/BC Processors

4.2.1.1 General Information--

The five ROM 2.1 IC/BC processors include P02G, P21G, P22G, P23G, and P24G. They have all been affected by changing CBM 4.0 to CBM 4.2 for ROM 2.1. Changes in the chemical species list (resulting in a net increase of five species) required modifying the processors' parameter statements that specify the number of species in array dimensions. The list of chemical reactions also changed, for a total of 83 reactions instead of CBM 4.0's 72 reactions. The changes in reactions affected only the three IC/BC processors that use the GPRIME set of algorithms (see Section 4.1.2.1) to equilibrate gas-phase chemistry (P21G, P23G, and P24G). Processor P21G uses GPRIME to equilibrate tropospheric background concentrations for all species. Next, processor P24G uses GPRIME to equilibrate observed ozone values with the background concentrations. Finally, P23G uses GPRIME to equilibrate background concentrations with a fixed value of ozone, to form the model's upper-boundary-condition concentrations (C-infinity). We designed GPRIME to work in all three processors so that the code could be maintained more easily and future changes to the chemical mechanism would affect only one set of routines.

Sections 4.2.1.2 through 4.2.1.6 discuss the IC/BC processors individually and list additional changes made to each one.

4.2.1.2 Processor P21G (Stage 0)--

In ROM 2.0, a program known as the independent chemistry module (ICM) equilibrated mean tropospheric concentrations of gases, taken from the literature (Table 3), and computed daytime and nighttime tropospheric background (clean-air) concentrations for each layer for all chemical species in the CBM 4.0 mechanism. For ROM 2.1, in order to standardize processing, we converted the ICM into processor P21G and added it to the processor network. P02G, P23G, and P24G all use the background concentrations P21G produces.

Processor P21G equilibrates gases using constant daylight photolysis rates for 720 min (12 h); daytime background concentrations are output after 600 min. The simulation continues, using constant nighttime photolysis rates for another 720 min, to total 1440 min (24 h); nighttime background concentrations are output after 1320 min.

TABLE 3. MEAN TROPOSPHERIC CONCENTRATIONS FOR ROM 2.1 SPECIES

Species*	Concentration (ppm)	Species*	Concentration (ppm)
Carbon monoxide (CO)	0.1	High molecular weight aldehydes (RCHO, R > H)	1.12×10^{-3}
Nitrogen dioxide (NO_2)	0.001	Formaldehyde (CH_2O)	1.4×10^{-3}
Nitric oxide (NO)	0.001	Toluene ($C_6H_5CH_3$)	1.4×10^{-4}
Ethene ($CH_2=H_2C$)	3.5×10^{-4}	Xylene ($C_6H_4(CH_3)_2$)	1.05×10^{-4}
Olefinic carbon bond (C=C)	2.1×10^{-4}	Paraffinic carbon bond (C-C)	7.42×10^{-3}

Source: Killus and Whitten (1984)

*All CBM 4.2 species not listed have values near zero; the model uses a value of 10^{-16} ppm.

4.2.1.3 Processor P02G (Stage 1)--

Processor P02G creates the ICON file, which contains the gridded initial-condition concentrations for each layer and species simulated by the core model. Because the first hour of any ROM simulation is the noon hour, P02G writes to the ICON file only the *daytime* background concentrations prepared by processor P21G. For each species, all cells in the grid are initialized with the same concentration value.

Except for standardizing the code, we made only one minor change to processor P02G for ROM 2.1: When P02G writes the ICON file header containing information on the file's contents, it uses the new header format required by the core model (see Section 3).

4.2.1.4 Processor P23G (Stage 1)--

(Note: Although we consider processor P23G an IC/BC processor, we included it in the meteorology section of Figure 4 because it does not directly result in the ICON file or BCON file.)

Processor P23G writes a file containing the hourly gridded upper-boundary-condition concentrations (C-infinity) used by the core model. This processor reads in the daytime and nighttime tropospheric background concentrations of all species for each layer, produced by processor P21G. P23G replaces the background ozone concentration with a value of 40 ppb, and then re-equilibrates all the species with this new ozone value. The daytime re-equilibrated concentrations are used to represent the C-infinity condition. However, the C-infinity file does not contain individual values for every CBM 4.2 species. Instead, based on an order-of-magnitude analysis of the C-infinity values, we have clustered all the CBM 4.2 species into 12 groups; all species in a group have values of the same order of magnitude. P23G averages the concentrations for all species in a group and uses the 12 averages to represent all species. The same C-infinity values are used for all hours of a model execution.

We made several changes to processor P23G for ROM 2.1: (1) Background concentrations are now equilibrated with an ozone level representative of the top boundary of the model; in ROM 2.0, no equilibration was attempted. Equilibrating concentrations can reduce the model's computation time when boundary fluxes are prevalent. (2) ROM 2.0 used 13 species to represent all CBM species; ROM 2.1 uses only 12. (3) The value representing each species group is now an average for all species in that group, rather than the actual concentration value for a selected species in each group.

4.2.1.5 Processor P24G (Stage 1)--

For each layer, processor P24G equilibrates background concentrations of all model chemical species with averaged observed ozone concentrations it reads in for the four domain boundaries, for both daytime and nighttime conditions. P22G uses this information to create the north, south, east, and west boundary-condition concentrations needed by the core model.

The changes made to processor P24G were based on a new data segregation. For a 1985 episode we have modeled in the ROMNET domain, we found a statistically significant difference between the western-boundary and southern-boundary daytime ozone average values, for over half of the episode days. We therefore decided to spatially segregate the western and southern daytime data. Then, because few ozone data were available for the northern and eastern boundaries, we used the minimum of the western and southern daytime values for these areas. We chose the minimum because the northern and eastern borders are removed from urban influences and so will likely have lower ozone concentrations than the western and southern borders.

We changed P24G to allow it to operate on the new set of ozone data. The ROM 2.0 version of P24G used the same boundary-condition concentrations for all four domain boundaries. The ROM 2.1 P24G instead calls GPRIME four times and produces one set of boundary-condition concentrations for each boundary.

4.2.1.6 Processor P22G (Stage 2)--

Processor P22G creates the BCON file, which contains the gridded boundary-condition concentrations for each species, layer, and advection time step modeled, for the domain's northernmost and southernmost grid cell rows and easternmost and westernmost grid cell columns. P22G reads in boundary-condition concentrations from processor P24G. Thus, when we changed P24G for ROM 2.1, we also had to change P22G to read in four sets of boundary conditions instead of just one set. Also, we changed P22G in the same way as P02G (which writes the ICON file), to write the BCON file header in the new format required by the core model.

4.2.2 Meteorology Processors

The 20 ROM 2.1 meteorology processors include P01G, P03G, P04G, P05G, P06G, P07G, P08G, P09G, P11G, P12G, P15G, P16G, P17G, P19G, P25G, P29G, P32G, P38G, P39G, and P40G. We consider processor P23G an IC/BC processor, so we have already discussed it above. It is included in the meteorology section of Figure 4 because it does not directly result in the ICON file or BCON file.

4.2.2.1 Processor P06G (Stage 0)--

Processor P06G computes the smoothed terrain elevation for each 10′ lat. by 15′ long. ROM domain grid cell, and also for a larger domain that extends three grid cells beyond the ROM domain. In addition, it computes average terrain elevations in a fine -resolution domain (cells 5′ lat. by 5′ long.) for the terrain penetration calculation. Finally, it computes the north-south and east-west components of the terrain elevation gradient (slope). Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.2.2 Processor P25G (Stage 0)--

Processor P25G computes the fraction of each grid cell in each land use category recognized by the model; it currently uses ten categories. Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.2.3 Processor P03G (Stage 1)--

Processor P03G prepares surface meteorology data (e.g., mixing ratio, virtual temperature, and wind speed) for use in higher-stage processors. We changed this processor for ROM 2.1 by adding the ability to estimate the occurrence of nighttime inversions on a local (grid cell by grid cell) basis.

4.2.2.4 Processor P16G (Stage 1)--

Processor P16G interpolates between rawinsonde observations to produce hourly upper-air profiles at 25-mb resolution, for use in higher-stage processors.

In creating the ROM 2.1 version from the 2.0 version, we changed the gridding methodology. P16G now spatially smooths the upper-air data using a Barnes-type analysis[2] that is point-specific, whereas the ROM 2.0 version smoothed by Barnes-gridding the data and then interpolating them back to the original data points using an overlapping quadratic surface fit. We implemented the new smoothing method because it performs the same basic function as before in a cleaner, more straightforward manner without oversmoothing the data.

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[2] The ROM uses several 2-D spatial analysis subroutines based on an objective analysis technique developed by Barnes (1973). Our application of this technique has been to use weighted averaging of the data to create gridded data from nongridded data.

Also, the ROM 2.0 P16G could read in data for nonstandard rawinsonde launch times, because such data were available for 1980. The ROM 2.1 version assumes that input data are available only at standard launch times. This change was data-driven and effectively simplifies the code. In addition, P16G can now accept surface meteorology station identification codes in either Weather-Bureau-Army-Navy (WBAN) format or call-letter format.

4.2.2.5 Processor P19G (Stage 1)--

Processor P19G computes hourly gridded values of fractional sky coverage at the terrain surface for all cloud types combined. Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.2.6 Processor P23G (Stage 1)--

This processor is discussed in Section 4.2.1.4.

4.2.2.7 Processor P01G (Stage 2)--

Processor P01G interpolates profiles of upper-air meteorological parameters at intervals of 50 m from hourly rawinsonde vertical profiles produced by P16G. Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.2.8 Processor P04G (Stage 2)--

The ROM 2.0 version of processor P04G computed gridded surface roughness (z_o) and hourly gridded Monin-Obukhov length (L), surface heat flux (Q), and friction velocity (u_*). The new ROM 2.1 P04G also writes hourly gridded files of surface temperature, surface relative humidity, and surface wind speed.

We upgraded P04G for ROM 2.1 by adding new procedures for estimating the meteorological parameters over large bodies of water. The ROM 2.1 version of P04G reads raw buoy-data files containing water surface and ambient air temperatures and wind speed. It then uses a three-step procedure to estimate L, Q, and u_* values over water: (1) it computes L, Q, and u_* at the buoys' locations and grids them for the whole domain; (2) it estimates these parameter values at each grid cell as it did in the ROM 2.0 version; and (3) it computes corrected parameter values

using an exponential weighting function that favors step 1's values more as the grid-cell-to-buoy-station distance decreases. For model episodes that lack buoy data with sufficient temporal resolution, P04G uses a file containing buoy data averaged for the episode month.

4.2.2.9 Processor P05G (Stage 2)--

Processor P05G uses surface observations to compute hourly gridded values for the fraction of sky covered by cumulus clouds, and also calculates cumulus cloud-top heights. Other than standardizing the code, we made no changes to this processor except a modification that allows it to accept surface meteorology station identification codes in either WBAN or call-letter format.

4.2.2.10 Processor P07G (Stage 3)--

Processor P07G computes hourly gridded wind fields in the cold layer (i.e., wind fields for layer 1 during inversion conditions), hourly gridded terrain penetration fractions, hourly gridded cold layer growth rates, and hourly gridded thicknesses for layers 0 and 1. Other than standardizing the code, we changed P07G only to correct a coding error that caused the magnitudes of the computed cold-layer winds to be in error by about 20%.

4.2.2.11 Processor P08G (Stage 4)--

Processor P08G computes hourly gridded cell thicknesses for layers 2 and 3, and various parameters used to specify volume fluxes between these two layers. We made several changes to produce the ROM 2.1 version. The ROM 2.0 P08G computed layer 1, 2, and 3 divergence fields used in wind fields processing; for ROM 2.1, we transferred this function from P08G to P11G. Also, in ROM 2.1's P08G, the top of layer 2 is gridded with respect to ground level instead of sea level, to avoid very thin layer 2 thicknesses over mountainous regions. In addition, P08G has been upgraded to accept surface meteorology station identification codes in either WBAN or call-letter format.

4.2.2.12 Processor P09G (Stage 5)--

Processor P09G computes hourly gridded atmospheric density, temperature, cloud cover, solar zenith angle, and water vapor concentration. The ROM 2.0 version of P09G used the Barnes gridding routine BGRID2 to produce a coarse grid, and then refined that grid to a regional grid

level using an overlapping quadratic routine. The ROM 2.1 P09G now uses the BGRID3 routine for all its gridding, thereby eliminating the coarse grid step. Also, because ROM 2.1 uses water vapor concentration in adjusting its CBM 4.2 reaction rate constants, P09G's output now includes values for this variable.

4.2.2.13 Processor P11G (Stage 5)--

Processor P11G computes hourly gridded horizontal winds for each layer, using rawinsonde vertical profiles and surface-station wind observations. P11G computes layer-averaged winds at rawinsonde sites and supplements these using layer averages extrapolated over surface weather station sites. It then uses Fourier series techniques to compute wind fields that fit these data and that satisfy mass balance and energy criteria known to exist in atmospheric flows. We have made substantial changes to this processor for ROM 2.1:

- In computing layer averages from rawinsonde profiles, we now use a height-dependent weighting scheme to better represent the pollutant transport patterns in layers 2 and 3.
- In ROM 2.0, surface-station data were rotated through "shear angles" representing the variation in wind direction with altitude, in order to obtain estimated layer averages for layers 1 and 2. The shear angles were computed using information in vertical profiles from nearby rawinsonde sites. The ROM 2.1 version of P11G incorporates scaling factors in the shear transformations in order to model the variations in both wind speed and direction with altitude. Surface data are used to represent the layer 1 average.
- P11G now computes divergence fields for layers 1, 2, and 3. In ROM 2.0, P08G performed this function. Also, the algorithm for layer 1 divergences now incorporates surface data, in addition to the vertical-profile rawinsonde data used by the older P08G version of the algorithm.
- We incorporated into P11G two other ROM 2.0 processors. In ROM 2.0, P11G received input files from processors P18G and P20G. Processor P18G created files containing two matrices used by P11G to transform equations describing physical wind field observations into equations for coefficients of the Fourier transform of the wind field. Processor P20G created a file containing the divergence transform matrix needed by P11G. In upgrading to ROM 2.1, we changed P18G and P20G from separate processors into P11G subroutines, and eliminated the intermediate files produced by P18G and P20G. All matrices are now created by P11G and stored in memory, rather than pre-computed by P18G and P20G, which enhances P11G's performance substantially.

- We corrected three errors that we found in the ROM 2.0 processors, one in P11G and two in P20G. The P11G subscripting error affected the computation of the divergent part of the wind field. The first P20G error occurred in the section that computes the imaginary part of the coefficient matrix. The second error in P20G, a missing EQUIVALENCE statement, prevented P20G from writing the imaginary part of the coefficient matrix; as a result, P11G was reading in a block of zeros instead of the actual coefficient values. Overall, correcting these errors resulted in winds having less of a westerly component and having somewhat higher energy.

4.2.2.14 Processor P17G (Stage 5)--

Processor P17G computes hourly gridded elevations (above MSL) for the tops of layers 0, 1, 2, and 3, and local time derivatives of these elevations. Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.2.15 Processor P32G (Stage 5)--

Processor P32G calculates hourly gridded horizontal eddy diffusivities for layers 1, 2, and 3, and also produces parameter fields needed to compute interfacial volume fluxes across layer boundaries. Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.2.16 Processor P12G (Stage 6)--

Processor P12G computes hourly gridded volume fluxes through all model layer boundaries, and cumulus cloud vertical flux parameters. Upgrades for ROM 2.1 did not involve methodology changes, but rather changes in the processing procedure.

P12G uses one of two different schemes for dealing with volume fluxes, depending on whether or not there is a nighttime inversion in layer 1. For ROM 2.1, we changed the gridded inversion indicator file written by P03G and read by P12G, so we also had to change the P12G mechanism that decides which volume flux scheme to use. In addition, we substantially improved and optimized P12G's code; it now runs faster than the ROM 2.0 version.

4.2.2.17 Processor P15G (Stage 6)--

Processor P15G computes hourly gridded deposition velocities for a set of representative species. ROM 2.0 computed deposition velocities for the following seven species:

- High molecular weight aldehydes (RCHO, R > H)
- Acetate (C_2O_3)
- Carbon monoxide (CO)
- Hydrogen peroxide (H_2O_2)
- Nitrous acid (HNO_2)
- Nitrogen dioxide (NO_2)
- Ozone (O_3)

It used these seven species to characterize the deposition velocities of the full set of ROM 2.0 (CBM 4.0) species. To calculate deposition velocity, P15G used raw data on land use and the presence or absence of salt water, relative humidity, Monin-Obukhov length, surface roughness length, friction velocity, and specified species-dependent deposition resistances. Due to a lack of suitable data, P15G assumed that deposition resistances for all the species were directly related to ozone deposition resistances.

We upgraded P15G for ROM 2.1 by including improved parameterizations for species-dependent deposition resistances (Wesely, 1988), which include variables such as solar irradiation, surface air temperature, molecular diffusivities and Henry's Law constants for the modeled species, reactivity factors for oxidation of biological substances, and surface wetness due to dew. P15G now requires input data on surface temperature, Monin-Obukhov length, surface roughness length, friction velocity, surface heat flux, land use fraction, solar zenith angle, a cloud cover correction factor, surface-layer relative humidity, and categories describing the seasonal characteristics of the modeled region. Due to the lack of solar irradiation and surface wetness data, P15G calculates values for these variables. Solar irradiation is determined using the method of Kondratyev (1969); surface wetness is determined by comparing the saturation specific humidity at the ground surface temperature (Deardorff, 1978) with the atmospheric surface-layer specific humidity.

The number of species that can be modeled by Wesely's method is limited only by the availability of Henry's Law constant data and reactivity factor data. As a result, processor P15G for ROM 2.1 calculates deposition velocities for ten representative species instead of seven:

- High molecular weight aldehydes (RCHO, R > H)
- Carbon monoxide (CO)
- Hydrogen peroxide (H_2O_2)
- Nitrous acid (HNO_2)

- Nitrogen dioxide (NO_2)
- Ozone (O_3)
- Formaldehyde (CH_2O)
- Nitric acid (HNO_3)
- Nitric oxide (NO)
- Peroxyacyl nitrate [$CH_3C(O)O_2NO_2$]

As with the ROM 2.0 species, the ten ROM 2.1 species are used to characterize the deposition velocity behavior for all species in the model.

4.2.2.18 Processor P29G (Stage 6)--

Processor P29G computes hourly gridded 30-min backtrack (advection) cell locations and horizontal diffusivities for each layer simulated by the core model. Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.2.19 Processor P38G (Stage 7)--

Processor P38G is a new processor developed for ROM 2.1 that reads the backtrack and diffusivity hourly gridded MF files output by P29G and computes the BTRK file parameters for each advection time step simulated by the core model. In ROM 2.0, this function was performed by processor P28G, which wrote the ROM 2.0 BMAT file. P28G does not exist in ROM 2.1.

4.2.2.20 Processor P39G (Stage 7)--

Processor P39G is also a new processor created for ROM 2.1 that reads all meteorology hourly gridded MF files *except* the backtrack and diffusivity files read by P38G and then computes the intermediate meteorology (IMET) file parameters for each advection time step simulated by the core model. ROM 2.0's P28G, which does not exist in ROM 2.1, performed the combined functions of P39G and P40G (below).

4.2.2.21 Processor P40G (Stage 8)--

Processor P40G is another new processor for ROM 2.1. It reads the intermediate meteorology (IMET) file produced by P39G and the emissions sources hourly gridded MF files produced by

P10G and computes the ROM 2.1 BMAT file parameters for each advection time step simulated by the core model. These functions were performed in ROM 2.0 by processor P28G.

4.2.3 Emissions Processors

The ROM 2.1 emissions processing system includes nine processors--P10G, P13G, P14G, P26G, P31G, P33G, P34G, P36G, and P41G--and the Biogenic Emissions Inventory System (BEIS).

4.2.3.1 Raw Emissions Data Processing--

In addition to upgrading the emissions processors for ROM 2.1, we also have created a set of routines that preprocess the emissions data before they reach the processor network. These ROM 2.1 preprocessing routines, described below, reduce file sizes and therefore computation time by eliminating emissions species that were carried along through the ROM 2.0 processor network even though they were not used by the core model.

NAPAP annual point-source emissions data--The NAPAP annual point-source emissions files contain data on 23 emissions species; the ROM uses only 14 of these. This file also contains daily and hourly allocation factors for each season of the year. We first use the VAX system sort to sort this annual file by state, county, plant, and point-source code. Next, because the ROM currently is run only for summer months and with only 14 of the species, we use the processing routine PTEXTR to extract only the necessary data from this annual file. PTEXTR outputs annual data with seasonal, daily, and hourly allocation factors for a given season. PTEXTR must be able to process NAPAP point-source input files with at least two different data formats, because the 1980 format is different from the 1985 format.

The 1985 point-source emissions data require a second raw data processing routine because the U.S. and Canadian data are in two separate files. This routine, PTMERG, simply combines the Canadian and U.S. data and is run before sorting the annual data file.

NAPAP area-source emissions data--When we receive them, the NAPAP area-source emissions data are hourly data sorted by season, and so do not require further temporal allocation. However, as with the point-source data, some of the area-source data contain emissions species not used in the ROM. The area-source data are first sorted by hour using the VAX system sort.

There are three files for each season: one for weekday emissions data, one for Saturday data, and one for Sunday data. We then run only the NAPAP 1980 data files through the routine AREXTR, which extracts the species data needed by the core model (NO_x, hydrocarbons, and CO) and outputs species, grid cell, and hour information to three individual output files (according to day type).

The 1985 data files are not run through AREXTR because they are already in the proper format. However, as with the point-source data, the 1985 area-source emissions data require another raw data processing routine because the U.S. and Canadian data are in two separate files. We run this routine, ARMERG, after both sets of data have been sorted; it simply combines the Canadian and U.S. data.

NAPAP mobile-source emissions data--The NAPAP mobile-source data are currently available only for 1985 and are in two separate data files, one for Canada and one for the U.S. As with the area-source data, there are three separate files for each season (a weekday file, a Saturday file, and a Sunday file). The two sets of mobile-source files are run through the routine MBMERG to combine the Canadian and U.S. data. We then use the VAX system sort to sort the three output files by hour and by state/county code. The mobile-source emissions files contain data that are not processed by the ROM system. We eliminate these data using the routine MBEXTR, which outputs only the data required by the mobile-source processor P26G. Processor P26G also requires input data on gridded daily average temperature and gridded daily temperature range (maximum minus minimum). We use the routine TEMPROC to generate a file with these data. This routine can process up to 72 days of data at one time, so we run it only once for each season.

After all the above raw data processing steps are completed, the point-, area-, and mobile-source emissions data are in a compact, more easily managed form and are ready for input to the processor network. The emissions processors are described below.

4.2.3.2 Processor P13G (Stage 0)--

Processor P13G computes the total length of all line emissions sources (highways and railroads) within each grid cell. Except for code standardization, we made no changes to this processor for ROM 2.1.

4.2.3.3 Processor P31G (Stage 0)--

Processor P31G allocates annual point-source emissions data between a weekday-emissions file, a Saturday-emissions file, and a Sunday-emissions file.

Most of the P31G changes made in converting it for ROM 2.1 were caused by input data format changes, as described in Section 4.2.3.1. The annual point-source data now are windowed for a particular season during raw data processing, so P31G no longer performs this task. Also, P31G no longer writes the data file containing the major point-source stack parameters because this is done in earlier raw data processing. We made these changes to streamline the point-source emissions data processing. In addition, we included methanol in the list of species P31G can process.

4.2.3.4 Processor P34G (Stage 0)--

Processor P34G converts all point-, area-, and mobile-source data files from Greenwich mean time (GMT) to local standard time (LST). It performs this time shift simply by reordering the data so that a given hour in GMT is written out as a different hour in LST.

We changed P34G for ROM 2.1 to include mobile-source emissions data in the time-shifting process. This was unnecessary in ROM 2.0 because mobile-source data were not separately available. We also added methanol to the list of species P34G can process.

4.2.3.5 Processor P36G (Stage 0)--

Processor P36G is a new processor designed for ROM 2.1. It applies NO_x and VOC emission controls at the county level for area- and mobile-source emissions data. The ROM 2.0 processor P35G, which does not exist in ROM 2.1, performed this function previously. P36G is run at an earlier stage than P35G was, and it allows emission controls to be applied and verified more accurately.

P36G applies area-source controls in a way similar to P35G's method, using a county-to-grid allocation file to relate each grid cell to a specific county. The major difference between the two processors is that P36G processes mobile-source data as well as area-source data. Because the

mobile-source data are already sorted by county as well as by grid cell, P36G applies controls to these sources directly, rather than having to go through the intermediate county allocation step described above for area sources.

4.2.3.6 Processor P41G (Stage 0)--

Processor P41G also is a new processor developed for ROM 2.1. It applies NO_x and VOC emission controls to point-source emissions data at a state, county, point, or individual-boiler (source classification code) level; the level of controls is specified in the control data file. The ROM 2.0 processor P35G performed this function previously. Because P41G is run at an earlier stage than P35G was, it allows specific emission controls to be applied and verified more accurately, and allows us to include additional options such as the ability to generate state and Consolidated Metropolitan Statistical Area summaries. P35G did not include the option of applying state-level controls.

4.2.3.7 Processor P26G (Stage 1)--

Processor P26G is another new processor for ROM 2.1. It computes hourly gridded mobile-source VOC, NO_x, and CO emissions parameters, adjusted for daily average temperature. In ROM 2.0, mobile sources were not treated separately from area sources. The two source types have been separated for ROM 2.1 because mobile-source emissions vary widely with local temperature, while other area-source emissions do not.

As discussed in Section 4.2.3.1, we use the routine TEMPROC during raw emissions data preprocessing to generate a file containing gridded daily average temperatures and daily temperature ranges for the ROM domain (in this case, days are measured from midnight to midnight), based on hourly surface meteorological and buoy temporal data. P26G then reads this file, adjusts hydrocarbon, NO_x, and CO emissions for temperature variation by applying algorithms to base gasoline and diesel exhaust emissions rates and to evaporative emissions rates, and applies emission rate adjustment factors based on estimated state motor vehicle inspection and maintenance program efficiencies (where such data are available). These adjustment factors also account for running loss and emission factor differences between Mobile 3.0 and Mobile 3.9, two versions of

the EPA Office of Mobile Sources algorithm used to estimate emissions from motor vehicles. P26G writes an hourly gridded file that contains the temperature-adjusted mobile source VOC, NO_x and CO emissions required by the core model.

4.2.3.8 Processor P14G (Stage 2)--

For a specific emissions scenario or time period, processor P14G prepares files containing hourly emissions values and stack descriptions for all major point sources, and combined hourly gridded emissions values for minor point sources, area sources, and mobile sources. It uses the weekday, Saturday, and Sunday emissions files to produce day-dependent data files for a specific 72-hour period (e.g., from noon on Thursday, July 17, 1980, through noon on Sunday, July 20, 1980).

For ROM 2.1, we changed the ROM 2.0 version to allow mobile-source data and area-source data to be input as separate files. P14G then merges these two files by summing mobile-source and area-source values for each species common to both files. Because the mobile-source data are already scenario-specific at this stage, P14G merges the data after it has processed the area-source emissions. In addition, we included methanol in the list of species P14G can process.

4.2.3.9 Processor P33G (Stage 6)--

Processor P33G generates hourly gridded locations and strengths of constant-source emitters for a tracer emissions species. We changed this processor for ROM 2.1 only by adding methanol to the list of species it can process, and by standardizing its code.

4.2.3.10 Processor P10G (Stage 7)--

Processor P10G computes hourly gridded emissions source functions in layers 0, 1, and 2 for combined anthropogenic and biogenic sources, and also computes the plume volume fraction in layer 0. The allocation between layers is based on layer heights, thicknesses, terrain penetration, and other meteorological variables, as well as on plume height for the point-source emissions. Most of the area-source emissions are found in layer 0.

In ROM 2.1, P10G makes better use of the terrain penetration factors to compute cell volumes and source strengths in each of the model layers. Also, we eliminated the option to include hazardous waste treatment, storage, and disposal facility (TSDF) data because hydrocarbon emissions from TSDFs are now included in the 1985 NAPAP emissions inventory. If necessary, however, this option can be reinstated in P10G with little difficulty. Finally, we added methanol to the list of species P10G can process.

4.2.3.11 The Biogenic Emissions Inventory System (BEIS) (Stage 6)--

In ROM 2.1, the BEIS prepares hourly gridded biogenic emission rates for the CBM 4.2 species isoprene, paraffin, olefin, high molecular weight aldehydes (RCHO, R > H), nonreactive hydrocarbons, NO, and NO_2. There are major differences between the ROM 2.0 and ROM 2.1 biogenic emissions processing.

ROM 2.0 biogenic emissions processing--ROM 2.0 processed biogenic hydrocarbon emissions in two stages. First, an external program called the Biogenic Emissions Software System (BESS) used land use, crop yield, and biomass density data to generate biogenic emission rates for nine roughly-defined classes of hydrocarbon emissions. Processor P27G then used these gridded emission rates to compute emission rates for the carbon bond species isoprene, paraffin, olefin, and methane.

In developing the BESS, Novak and Reagan (1986) gathered three types of information: (1) emission factors for vegetation indigenous to the eastern U.S.; (2) empirical relationships between these emission factors and temperature and solar intensity; and (3) gridded estimates of biomass density for each vegetation species. The BESS computed biogenic hydrocarbon emission rates for each vegetation species by adjusting the emission factors using hourly temperature and solar intensity data and then multiplying the hourly emission factors ($\mu g/g/h$) by the gridded species biomass (g dry foliar weight). Hydrocarbon emissions were divided into nine categories:

(1) Isoprene only (mol/h)

(2) Monoterpene only (mol/h)

(3) Total nonmethane hydrocarbon (TNMHC) (mol/h)

(4) Methane (mol/h)

(5) TNMHC without monoterpene and isoprene (g/h)

(6) TNMHC with monoterpene and possibly with isoprene (g/h)

(7) TNMHC with isoprene and possibly with monoterpene (g/h)

(8) TNMHC without isoprene but possibly with monoterpene (g/h)

(9) TNMHC with monoterpene but possibly without isoprene (g/h)

Obviously, several of the categories are defined rather imprecisely, due primarily to a lack of the speciated chemical measurements used in developing the biogenic emission factors. To circumvent these uncertainties, EPA atmospheric chemists devised a system allocating each of the nine categories' emission rates between three categories: isoprene, monoterpene, and methane. Table 4 shows the distribution assumed in ROM 2.0.

Next, P27G determined a final emission rate for each of the three categories by summing all rates for that species from the nine categories. Finally, the emission rates for isoprene, monoterpene, and methane were split into final hourly gridded emission rates for the four ROM 2.0 carbon bond classes and written to a ROM data file, based on the following allocations:

- 1 mol isoprene was treated as 1 mol isoprene and 1 mol paraffin
- 1 mol monoterpene was treated as 1 mol olefin and 8 mol paraffin
- 1 mol methane was treated as 0.99 mol methane and 0.01 mol paraffin

ROM 2.1 biogenic emissions processing--We have designed the new biogenic emissions processing system, the BEIS, so that both ROM 2.1 and the Regional Acid Deposition Model (RADM) can use it. The basic structure of the BEIS is similar to the combined BESS and P27G system used in ROM 2.0, but there are some major differences:

(1) The BEIS uses broad vegetation classes rather than the individual plant species used in the ROM 2.0 biogenic emissions processing, because outside the NEROS and SEROS model domains there is neither enough information on the regional distribution of individual plant species nor enough experimental data to determine how to allocate emission factors to individual species.

(2) The BEIS includes a canopy model for estimating leaf temperature and solar intensity profiles in forested areas; the ROM 2.0 P27G used no canopy model at all. The canopy model, developed by Dr. Brian Lamb of Washington State University (personal communication, 1989),

TABLE 4. FORMULAS USED FOR DERIVING EMISSION RATES FOR ISOPRENE, MONOTERPENE, AND METHANE, BASED ON THE NINE BESS HYDROCARBON EMISSIONS CATEGORIES

Hydrocarbon emissions category	Compound(s) within category	Formula used to calculate emission rate of compound within category*
1	Isoprene	$1.00 \cdot Cat_1 = Iso_1$
2	Monoterpene	$1.00 \cdot Cat_2 = Mono_2$
3	Monoterpene	$0.25 \cdot Cat_3 = Mono_3$
4	Methane	$1.00 \cdot Cat_4 = Meth_4$
5	Monoterpene	$0.25 \cdot Cat_5/MW_{mono} = Mono_5$
6	Isoprene	$0.20 \cdot Cat_6/MW_{iso} = Iso_6$
	Monoterpene	$0.575 \cdot Cat_6/MW_{mono} = Mono_6$
7	Isoprene	$0.50 \cdot Cat_7/MW_{iso} = Iso_7$
	Monoterpene	$0.275 \cdot Cat_7/MW_{mono} = Mono_7$
8	Monoterpene	$0.40 \cdot Cat_8/MW_{mono} = Mono_8$
9	Monoterpene	$0.625 \cdot Cat_9/MW_{mono} = Mono_9$

*Notes to column 3:

(1) Cat_n represents category n's emission rate. The units for Cat_n are mol/h if the formula does not include division by molecular weight; if this division is included, then the units for Cat_n are g/h.

(2) Iso_n, $Meth_n$, and $Mono_n$ represent emission rates for isoprene, methane, and monoterpene for category n; all of these rates are in mol/h.

(3) MW_{iso} represents the molecular weight of isoprene, assumed here to be 68 g/mol. MW_{mono} represents the molecular weight of monoterpene, assumed here to be 136 g/mol.

computes the leaf temperature and solar intensity at eight levels in deciduous and coniferous canopy types. This allows us to compute more accurately the temperature and solar intensity profiles within a tree canopy and to use these profiles with Tingey correction curves. ROM 2.0 did not model the temperature and solar intensity attenuations that result from canopy effects, which possibly caused the model to overestimate emission rates.

(3) The BEIS calculates emission rates directly for isoprene, α-pinene, monoterpene, and unknown species, rather than for the nine ROM 2.0 roughly-defined hydrocarbon classes. It then converts these into emission rates for the CBM 4.2 species isoprene, paraffin, olefin, high molecular weight aldehydes, and nonreactive hydrocarbons using the following allocations:

- 1 mol isoprene is treated as 1 mol isoprene
- 1 mol monoterpene or α-pinene is treated as 0.5 mol olefin, 6 mol paraffin, and 1.5 mol higher aldehydes
- 1 mol unknown species is treated as 0.5 mol olefin, 8.5 mol paraffin, and 0.5 mol nonreactive hydrocarbons.

(4) The BEIS calculates NO and NO_2 emission rates for grasslands using a temperature-sensitive algorithm suggested by F. Fehsenfeld of NOAA (personal communication, 1988)

(5) The BEIS is written in SAS (SAS Institute Inc., 1985) instead of FORTRAN. This has allowed us to improve quality assurance procedures and to interface the BEIS with both the ROM and the RADM. Because the BEIS is not written in FORTRAN, it cannot be run in the normal processor fashion and we did not give it a P*nn*G name.

4.3 PF/MF DATABASE CHANGES

We have modified the PF/MF database directory file, which controls the processors' access to the PFs and MFs, to reflect the addition of new 2.1 processors and PF/MF files, the deletion of several ROM 2.0 processors and PF/MF files, the modifications made in converting ROM 2.0 processors to ROM 2.1 processors, and the changes we made to the stage numbers of some processors as we incorporated them into the ROM 2.1 network.

Also, we have upgraded the PF/MF database software for ROM 2.1 by incorporating better error checking procedures. As it executes, it ensures that the PF/MF files used are the correct ones for the given region or application, by verifying that the region itself has been written into the internal header of the file and that the PF/MF file number falls within the limits defined for the application.

SECTION 5

SUMMARY OF THE DIFFERENCES BETWEEN ROM 2.0 AND ROM 2.1

We have discussed the many improvements made to the ROM in upgrading it from version 2.0 to version 2.1. It should now predict more accurately the ozone concentration changes that would result from specified emissions changes, and thus be a better tool for evaluating VOC and NO_x emission control programs. We have also designed version 2.1 so that future outside users will be able to apply the ROM more easily, and so that it makes more efficient use of computer resources. The first strategy-evaluation application of ROM 2.1 will be for EPA's Regional Ozone Modeling for Northeast Transport (ROMNET) project. Three types of emissions scenarios will be examined: base-year (1985) emissions, future-year (1995 and 2005) emission projections, and the effects of various control strategies on the projected emissions. The results will be used to assess the strategies' impacts on boundary conditions (for use in urban-scale modeling), regional ozone concentrations, and inter-urban transport.

This final section briefly lists the major differences between the 2.0 and 2.1 versions of the ROM. For more detailed information, please refer to Section 3 (core model changes) and Section 4 (processor network changes). Also, for a functional descriptions summary and schematic of the ROM 2.1 processor network, please refer to Figure 4 and Table 1 at the end of Section 2.

5.1 SUMMARY: CHANGES MADE TO THE CORE MODEL AND ITS INPUT FILES

To upgrade the ROM 2.0 core model and its input files for ROM 2.1, we made the changes described below in Sections 5.1.1 through 5.1.3.

5.1.1 ROM Chemistry Solver Changes

Overall, the changes shown below have increased the computation time for a core model run by about 54%, for a NEROS domain three-day execution on the IBM 3090.

- We implemented a more recent version of the Carbon Bond Mechanism, CBM 4.2; ROM 2.0 used CBM 4.0. CBM 4.2 includes a different chemical species list, a different list of chemical reactions and their rate constants, and it uses an additional variable, water vapor concentration, to adjust the reaction rate constants. (See Section 3.1.1.1.)

- Partly as a result of implementing CBM 4.2, we have altered the FRAX mechanism, which chooses the lengths of the model's chemistry time steps and controls the degree of solution accuracy for the chemical kinetics equations. Overall, the changes cause the model to choose shorter time steps more often than in ROM 2.0, resulting in increased computation time. However, we have offset this increase by changing the minimum allowable time step length from 10 s to 20 s. (See Section 3.1.1.2.)

- We have added methanol to the list of model species (in addition to the other species list changes caused by implementing CBM 4.2), so that ROM 2.1 can be used to evaluate ozone-reduction strategies involving choices between automotive fuels. (See Section 3.1.1.3.)

5.1.2 Core Model I/O Modifications to Improve Efficiency

- We have split the ROM 2.0 B-matrix (BMAT) file into two files, BTRK and the new BMAT. The BTRK file contains the backtrack and diffusivity information used by the core model's BIGGAM module; the new BMAT file contains the parameterization for vertical fluxes, the meteorological parameters necessary for chemistry rate constant adjustment, and parameterized emissions source strengths, all needed by the core model's LILGAM module. We also designed the new BMAT file to be a multiple BMAT file that can be distributed over many disks. (See Section 3.1.2.1.)

- We eliminated the row-windowing feature, which was included in ROM 2.0 because of memory limits on older computers. (See Section 3.1.2.2.)

5.1.3 Changes That Should Allow Future Outside Users to Apply the Core Model

- Eventually, we plan to release the core model to outside users so that they can perform their own emission control strategy evaluations. However, running the meteorology portion of the processor network to produce the BMAT and BTRK core model input files requires a huge amount of ADP resources and specialized processing by trained personnel. We have relieved future outside users of this burden by designing the ROM 2.1 processor network to produce one large file from stages 0 through 7 of the meteorology network, called the IMET file. We will provide users with an IMET file for each three-day episode they choose; they will run the

emissions portion of the processor network themselves to produce the final emissions MF files (from P10G), and then combine these MF files with our IMET file to produce their own BMAT file. We will also give them ICON, BCON, and BTRK files for each three-day episode, so that they will then have all four of the input files needed to run the core model. (See Section 3.2.)

In addition to the changes listed in the three subsections above, we also improved the core model by (1) reversing the vertical-layer-then-column order of BIGGAM's computations, (2) improving reporting to the run-time log file, (3) standardizing the code so that it is easier to read and to maintain, and (4) simplifying and standardizing the structure of the file headers that give information on the contents of each core model file. (See Section 3.1.3.)

5.2 SUMMARY: CHANGES MADE TO THE INPUT PROCESSOR NETWORK

5.2.1 ROM 2.0 Processors Deleted From the Network During the Upgrade

Overall, in converting from ROM 2.0 to ROM 2.1, we deleted five ROM 2.0 processors from the network and incorporated their functions into other processors:

- ROM 2.0's [P18G] and [P20G] have been incorporated into the ROM 2.1 version of P11G (the primary wind fields processor) as subroutines. (See Section 4.2.2.13.)
- The ROM 2.0 biogenic emissions processor, [P27G], has been replaced with the BEIS.
- The functions of ROM 2.0's [P28G], which wrote the ROM 2.0 BMAT file, are now included in the new ROM 2.1 processors P38G, P39G, and P40G, which write the ROM 2.1 BTRK and BMAT files. (See Sections 4.2.2.19, 4.2.2.20, and 4.2.2.21.)
- The functions of ROM 2.0's [P35G], which applied point- and area-source emissions controls, are included in the new ROM 2.1 processors P36G and P41G. (See Sections 4.2.3.5 and 4.2.3.6.)

5.2.2 ROM 2.1 Processors Added to the Network During the Upgrade

We also added seven new processors and the Biogenic Emissions Inventory System (BEIS) to the network in upgrading the ROM to version 2.1. Some of these perform functions that were included in ROM 2.0 processors we have deleted from the network (see above), and some perform functions not included in ROM 2.0's processor network at all.

- P21G equilibrates mean tropospheric concentrations of gases and computes daytime and nighttime tropospheric background (clean-air) concentrations for each layer for all chemical species in the CBM 4.2 mechanism. (See Sections 4.1.2.1, 4.2.1.1, and 4.2.1.2.)

- P26G computes hourly gridded mobile-source VOC, NO_x, and CO emissions parameters, adjusted for daily average temperature. (See Sections 4.2.3.1 and 4.2.3.7.)

- P36G applies NO_x and VOC emission controls at the county level for area- and mobile-source emissions data. (See Section 4.2.3.5.)

- P38G reads the backtrack and diffusivity hourly gridded MF files output by P29G and computes the BTRK file parameters for each advection time step simulated by the core model. (See Section 4.2.2.19.)

- P39G reads all meteorology hourly gridded MF files *except* the backtrack and diffusivity files read by P38G and then computes the intermediate meteorology (IMET) file parameters for each advection time step simulated by the core model. (See Section 4.2.2.20.)

- P40G reads the intermediate meteorology (IMET) file produced by P39G and the emissions sources hourly gridded MF files produced by P10G and computes the ROM 2.1 BMAT file parameters for each advection time step simulated by the core model. (See Section 4.2.2.21.)

- P41G applies NO_x and VOC emission controls to point-source emissions data at a state, county, point, or individual-boiler (source classification code) level. (See Section 4.2.3.6.)

- BEIS, the biogenic emissions processing system, is written in SAS instead of FORTRAN (see Section 4.2.3.11). It has replaced the ROM 2.0 combination of the BESS and P27G, and differs from it in the following ways:

  - In computing biogenic hydrocarbon emission rates, the BEIS uses broad vegetation classes instead of individual species.

  - It includes a canopy model that allows it to compute more accurately the temperature and solar intensity profiles within a tree canopy.

  - It calculates emission rates for isoprene, α-pinene, monoterpene, and unknown species (instead of for nine roughly-defined hydrocarbon classes), and then converts these into emission rates for the CBM 4.2 species isoprene, paraffin, olefin, high molecular weight aldehydes (RCHO, R > H), and nonreactive hydrocarbons.

  - The BEIS calculates NO and NO_2 emission rates for grasslands; P27G in ROM 2.0 did not output these species at all.

5.2.3 ROM 2.0 Processors That Are Included in the ROM 2.1 Network

Twenty-seven of the ROM 2.0 processors are also included in the ROM 2.1 processor network. Some are essentially unmodified, but all have been changed in minor or major ways. In addition to the changes listed below, the code for all processors has been standardized so that it is easier to read and to maintain. Also, we have completed enhancements to the network that allow us to model domains with dimensions other than 60 columns by 42 rows, and that allow us to apply the network more easily to different geographic regions (see Section 4.1.1).

We have modified the PF/MF database directory file, which controls the processors' access to the PFs and MFs, to reflect the changes we have made to the processor network for ROM 2.1. We have also upgraded the PF/MF database software by incorporating better error checking procedures. (See Section 4.3.)

In addition to upgrading processors, we have also created a set of raw data processing routines that preprocess the emissions data before they reach the emissions portion of the network. These routines reduce file sizes, and therefore computation time, by eliminating unnecessary parameters. (See Section 4.2.3.1.)

5.2.3.1 ROM 2.0 Processors That Did Not Change for ROM 2.1--

There were eight ROM 2.0 processors that we did not modify in converting to ROM 2.1, except in the general ways mentioned in the previous paragraph: P01G, P06G, P13G, P17G, P19G, P25G, P29G, and P32G. Their functions are described in Table 1.

5.2.3.2 ROM 2.0 Processors Altered for ROM 2.1--

We made minor or major modifications to 19 of the ROM 2.0 processors during the upgrade to ROM 2.1, in addition to the general changes we made to all processors. The items listed below are all differences between ROM 2.0 and ROM 2.1 versions of the processors.

- P02G processes the CBM 4.2 species instead of the CBM 4.0 species, and also writes the ICON file header in the new format required by the ROM 2.1 core model. (See Sections 4.1.2.1, 4.2.1.1, and 4.2.1.3.)

- P03G can now estimate the occurrence of nighttime inversions on a local (grid cell by grid cell) basis. (See Section 4.2.2.3.)

- P04G now writes hourly gridded files of surface temperature, surface relative humidity, and surface wind speed. We have also added new procedures that use buoy data to estimate meteorological parameters. (See Section 4.2.2.8.)

- P05G can accept surface meteorology station identification codes in either WBAN or call-letter format. (See Section 4.2.2.9.)

- We eliminated a coding error in P07G that caused the magnitudes of the computed cold-layer winds to be in error by about 20%. (See Section 4.2.2.10.)

- P08G no longer computes layer 1, 2, and 3 divergence fields used in wind fields processing; we transferred this function to P11G. Also, P08G now grids the top of layer 2 with respect to ground level instead of sea level. Finally, P08G can accept surface meteorology station identification codes in either WBAN or call-letter format. (See Section 4.2.2.11.)

- P09G uses an improved gridding method, and also outputs water vapor concentration values. (See Section 4.2.2.12.)

- P10G makes better use of terrain penetration factors to compute cell volumes and source strengths, and also includes methanol in the list of species it can process. In addition, we eliminated the option to include hazardous waste TSDF input data. (See Sections 4.1.2.2 and 4.2.3.10.)

- We made substantial changes to P11G (see Section 4.2.2.13):

  - P11G now uses a height-dependent weighting scheme to compute averages for layers 2 and 3 from rawinsonde profiles.

  - It includes scaling factors in shear transformations in order to model the variations in both wind speed and direction with altitude.

  - It now computes divergence fields for layers 1, 2, and 3; P08G performed this function in ROM 2.0. Also, the algorithm for layer 1 divergences now incorporates surface data, in addition to the vertical-profile rawinsonde data used by the older P08G version of the algorithm.

  - We have incorporated the ROM 2.0 processors P18G and P20G into P11G as subroutines.

  - We corrected three errors in the ROM 2.0 version; overall, these corrections resulted in winds having less of a westerly component and having somewhat higher energy.

- Because we changed the gridded inversion indicator file read by [P12G], we had to change the processor's mechanism for deciding which of two volume flux schemes to use. Also, we substantially improved and optimized P12G's code so that it runs noticeably faster than before. (See Section 4.2.2.16.)

- [P14G] now allows mobile-source and area-source data to be input as separate files; it also includes methanol in the list of species it can process. (See Sections 4.1.2.2 and 4.2.3.8.)

- [P15G] includes improved parameterizations for species-dependent deposition resistances, and models ten representative species instead of seven. (See Section 4.2.2.17.)

- To produce its upper-air profiles, [P16G] now uses an improved smoothing method that does not oversmooth the data. We have also eliminated the option to read in data for nonstandard rawinsonde launch times, and have modified P16G to accept surface meteorology station identification codes in either WBAN or call-letter format. (See Section 4.2.2.4.)

- [P22G] can now process the CBM 4.2 species. It also reads in four sets of boundary conditions instead of one, and writes the BCON file header in the new format required by the 2.1 core model. (See Sections 4.1.2.1, 4.2.1.1, and 4.2.1.6.)

- [P23G] now processes the CBM 4.2 species, and includes the GPRIME set of algorithms that is based on the CBM 4.2 ROM chemistry solver mechanism. In addition, P23G equilibrates background concentrations with an ozone level representative of the top boundary of the model. It also models 12 representative species instead of 13, and calculates the values for these 12 species a different way. (See Sections 4.1.2.1, 4.2.1.1, and 4.2.1.4.)

- Like P23G, [P24G] now processes the CBM 4.2 species and includes the GPRIME set of algorithms. It also produces four different sets of boundary conditions instead of just one. (See Sections 4.1.2.1, 4.2.1.1, and 4.2.1.5.)

- [P31G] no longer windows the annual point-source data for a particular season, and it no longer produces the data file containing the major point-source stack parameters; the new raw emissions data preprocessing routines perform both these functions. Also, P31G now includes methanol in the list of species it can process. (See Sections 4.1.2.2 and 4.2.3.3.)

- [P33G] can now process the species methanol. (See Sections 4.1.2.2 and 4.2.3.9.)

- [P34G] now includes mobile-source emissions in its time-shifting process, and it includes methanol in the list of species it can process. (See Sections 4.1.2.2 and 4.2.3.4.)

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